Stability and Anion Diffusion Kinetics of Yttria-stabilized zirconia Resolved from Machine Learning Global Potential Energy Surface Exploration

Shu-Hui Guan,[†,‡] Ke-Xiang Zhang[‡], Cheng Shang,[*,‡] and Zhi-Pan Liu[*,‡]

[†] Shanghai Academy of Agricultural Sciences, Shanghai 201403, China

[‡] Collaborative Innovation Center of Chemistry for Energy Material, Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Key Laboratory of Computational Physical Science, Department of Chemistry, Fudan University, Shanghai 200438, China

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1. Construction of Y-Zr-O ternary G-NN potential
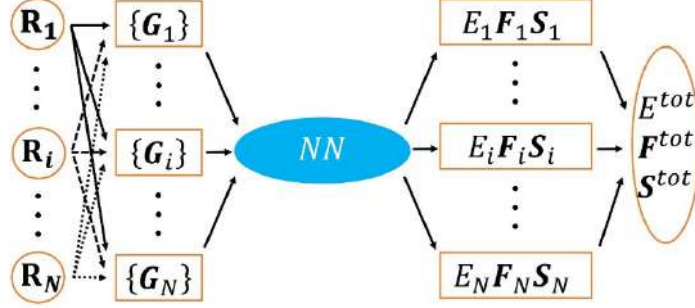
a. NN architecture

Figure S1 | Scheme for the HDNN architecture. The subscripts i and N represent atom indices and total number of atoms in a structure. The input of a NN is a set of structural descriptors $\{\mathbf{G}_i\}$ constructed from Cartesian coordinates $\{\mathbf{R}\}$ of a structure, and the outputs are the atomic properties $\{E_i, \mathbf{F}_i, \mathbf{S}_i\}$, i.e. energy, forces and stresses. The overall properties E^{tot}, $\mathbf{F}^{tot}$, and $\mathbf{S}^{tot}$, can be calculated from the individual atomic contributions.

In this work, we utilized the high dimensional neural network (HDNN) scheme to construct the NN potential[1, 2]. The NN architecture is schematically shown in Fig. S1. In Eq 1, the total energy E^{tot} can be decomposed and written as a linear combination of atomic energy E^i, which is the output of the standard neural network. The input nodes are a set of geometry-based structural descriptors, $\{\mathbf{G}_i\}$, and are very detailed discussed in main text.

$$E^{tot} = \sum_i E_i \, , (1)$$

The atomic force can be analytically derived according to Eq. 2, where the force component $F_{k,\alpha}$, α=x, y or z, acting on the atom k is the derivative of the total energy with respect to its coordinate $R_{k,\alpha}$. By combining with Eq. 1, the force component can be further related to the derivatives of the atomic energy with respect to j^{th} structural descriptors of atom i, $G_{j,i}$:

$$F_{k,\alpha} = -\frac{\partial E^{tot}}{\partial R_{k,\alpha}} = -\sum_{i,j} \frac{\partial E_i}{\partial G_{j,i}} \frac{\partial G_{j,i}}{\partial R_{k,\alpha}}, (2)$$

Similarly, the static stress tensor matrix element $\sigma_{\alpha\beta}$ can be analytically derived as:

$$\sigma_{\alpha\beta} = -\frac{1}{V}\sum_{i,j,d} \frac{(\mathbf{r}_d)_\alpha (\mathbf{r}_d)_\beta}{r_d} \frac{\partial E_i}{\partial G_{j,i}} \frac{\partial G_{j,i}}{\partial r_d}, (3)$$

where $\mathbf{r}_d$ and r_d are the distance vector constituting of $G_{j,i}$ and its module, respectively, and V is the volume of the structure.

b. Construction of the global dataset using SSW-NN

Undoubtedly, the dataset used for training the NN determines largely the quality of NN PES. Our previous work has shown that the stochastic surface walking (SSW) global optimzation[3, 4] can be used to fast generate a global dataset, which incorporates different structural patterns on the global PES. The details of SSW method can be found in the previous work. The SSW PES search is fully automated and does not need a priori knowledge on the system, such as the structure motif (e.g., bonding patterns, symmetry) of materials. The final obtained Y-Zr-O global dataset in this work is detailed in **Table S1**.

In brief, the SSW-NN method involves three stages for constructing the global dataset, as described in the following.

(i) **The first stage** constructs a raw dataset, which contains the most commmon atomic environment and serves as the training dataset for building an initial NN PES. This is done by performing first principles SSW global optimization in a massively parallel way. The first principles calculation is typically with low accuracy setups and restricted to small unit cells (typically below

79 atoms) to speed up the SSW search. By collecting and screening the structures from the SSW trajectories, a raw dataset is finally obtained.

(ii) **The second stage** trains an NN global PES. This is done by first refining the dataset using first principles calculation with high accuaracy setups, followed by the NN training on the accurate global dataset. The NN architecture applied in this stage utilizes a small set of structural descriptors and a small network size.

(iii) **The third stage** iteratively expands the global dataset. It targets to increase the predictive power of NN PES by incorporating more structural patterns into the dataset. This is done by carrying out SSW PES search using the NN PES obtained in the second stage, starting from a variety of initial structures. These initial structures are often randomly configurated and also include large systems with many atoms per unit cell (e.g. 158 atoms). The structures from all SSW trajectories are collected and filtered to genereate the addtional dataset. This new dataset is then fed to the global dataset (back to stage 2) to start a new cycle of NN training.
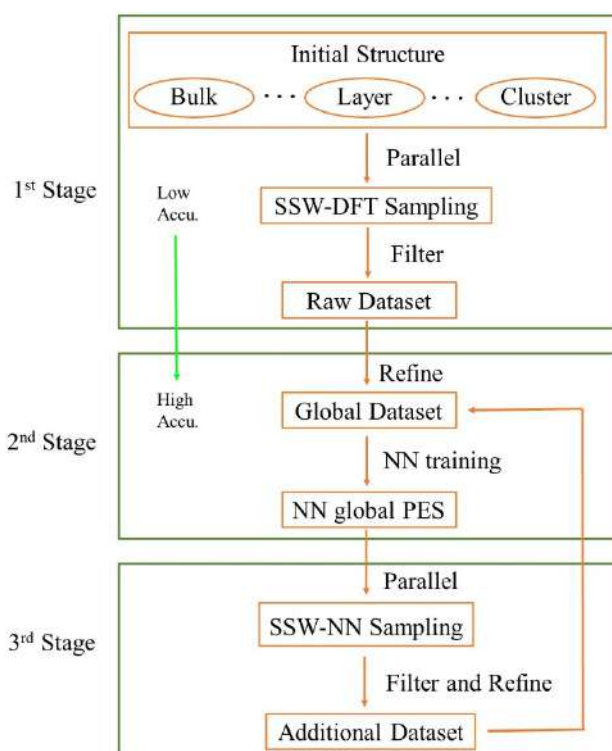
Scheme S1 | Procedure for generating the training dataset using SSW global optimization. At the first stage, the SSW sampling is typically calculated with low accuracy first principle calculations. At the second stage, the global dataset is first refined using high accuracy setups, followed by the NN training on the accurate global dataset. At the third stage, an additional dataset is generated by SSW sampling utilizing NN PES obtained previously. This additional dataset is then fed into global dataset (back to stage 2) and start a new cycle of NN training.

Table S1 | Structure information in the first principles global dataset. Listed data are the number of the structures in the global dataset, as distinguished by the chemical formula (Species), the number of atoms per cell (N_{atm}), the type of structures, being cluster (N_{cls}), layer (N_{lay}) and bulk (N_{bul}). Total number of structures (N_{tot}) are also summarized.

Species	N_{atm}	N_{cls}	N_{lay}	N_{bul}	N_{tot}
Zr8	8	0	13	97	110
Zr13	13	0	6	6	12
Zr16	16	1057	3	3616	4676
Zr21	21	0	3	1401	1404
Zr32	32	0	5	363	368
O1	1	2	0	0	2
O1-Zr12	13	0	995	0	995
O2-Zr8	10	0	57	202	259
O2-Zr10	12	0	541	0	541
O3-Zr18	21	0	134	67	201
O3-Zr49	52	0	25	9	34
O4	4	0	14	0	14
O4-Zr4	8	0	111	369	480
O4-Zr8	12	0	56	245	301
O4-Zr22	26	0	14	59	73
O5-Zr27	32	0	2	59	61
O6-Zr4	10	0	0	25	25
O6-Zr8	14	0	68	273	341
O6-Zr15	21	0	126	0	126
O6-Zr18	24	0	15	69	84
O7-Y2-Zr2	11	0	38	2020	2058
O8-Zr4	12	0	112	9379	9491
O8-Zr8	16	0	58	233	291
O8-Zr15	23	0	22	84	106
O10-Zr8	18	0	82	287	369
O10-Zr22	32	0	1	71	72
O11	11	0	73	22	95
O12-Zr8	20	0	0	245	245
O12-Zr40	52	0	8	0	8
O13-Zr7	20	0	24	10	34
O14-Zr8	22	0	0	118	118
O15-Zr9	24	0	1	184	185
O17-Zr16	33	0	21	1	22
O18-Zr12	30	0	219	10	229
O18-Zr40	58	0	67	1	68
O20-Zr38	58	0	36	2	38
O21-Y2-Zr9	32	0	0	21	21
O24-Y16	40	0	13	1037	1050

O26-Y12-Zr4	42	0	17	0	17
O27-Y10-Zr6	43	0	19	3	22
O28-Y8-Zr8	44	0	16	4	20
O29-Y6-Zr10	45	0	21	6	27
O30-Y4-Zr12	46	0	21	2844	2865
O31-Y2-Zr13	46	0	12	0	12
O31-Y2-Zr14	47	0	25	1026	1051
O31-Y3-Zr13	47	0	25	8	33
O32-Y2-Zr14	48	0	19	4	23
O42-Y4-Zr18	64	0	0	21	21
O52-Y4-Zr23	79	0	0	105	105
total	--	1059	3138	24606	28803

2. Definition of distance-weighted Steinhart order parameter

The distance-weighted Steinhardt-type order parameter[5] (OP) defined by Eq. 4 with the degree l=2,4, 6, as also utilized previously to distinguish the short-medium range ordering of solid structures.

$$OP_L = \left(\frac{4\pi}{2L+1} \sum_{m=-L}^{L} \left| \frac{1}{N_{bonds}} \sum_{i \neq j} e^{-\frac{1}{2}\frac{r_{ij}-r_c}{r_c}} Y_{Lm}(\boldsymbol{r}_{ij}) \right|^2 \right)^{\frac{1}{2}} \quad (4)$$

In Eq.4, Y_{Lm} is the spherical harmonic function, i and j are atoms in lattice, $\boldsymbol{r}_{ij}$ is the vector between the atom i and j, and r_{ij} is their distance; r_c is set as 60% of the typical single bond length for i and j atoms (e.g. ~2.5 Å for Zr-O bond); N_{bonds} is the number of bonds in the first bonding shell. By choosing a suitable degree, the order parameter can measure the short- and medium-range ordering of atoms in the lattice.

3. Benchmark of G-NN potential against DFT calculations

The performance of NN potential performance has been carefully benchmarked. We select 18 YZrO structures including GMs at different structures and transition state (TS) along the reaction pathway to compare the NN results with the DFT calculation results. It could be seen that the energy obtained from NN and DFT calculations is highly consistent and the difference of the energy is less than 2.4 meV/atom, which is quite standard for NN potentials and accurate enough for searching the stable candidates. The details for the comparison between DFT and NN results can be found in **Table S2**.

Table S2 | Benchmark of NN calculations for YSZ systems as compared with DFT results. Listed data includes the compositions, structure, DFT energy, NN energy and energy differences between DFT energy and NN energy (E_{diff}, meV/atom).

No.	Species	structure	E_{DFT}/eV	E_{nn}/eV	ΔE_{NN-DFT} /eV	ΔE_{NN-DFT} /(meV/atom)
1	Y2Zr14O31	GM (6.7YSZ)	-444.41202	-444.369121	0.0429	0.9127
2	Y2Zr14O31	GM-1 (6.7YSZ)	-443.94965	-443.874952	0.0747	1.5893
3	Y4Zr23O52	GM	-746.15531	-746.05458	0.1007	1.2751
4	Y4Zr23O52	Str-1	-745.92902	-745.951219	-0.0222	-0.281
5	Y4Zr23O52	Str-2	-745.84421	-745.798775	0.04544	0.5751
6	Y4Zr23O52	Str-3	-745.75803	-745.714432	0.0436	0.5519
7	Y4Zr18O42	GM(10YSZ)	-604.39926	-604.246797	0.1525	2.3822
8	Y4Zr12O30	GM(14.3YSZ)	-433.95425	-433.863222	0.09103	1.9789
9	Y8Zr16O44	GM(20YSZ)	-320.37845	-320.294985	0.08347	1.2274
10	Zr8Y8O28	GM(33.3YSZ)	-411.67895	-411.581107	0.09784	2.2237
11	Zr9Y12O36	GM(40YSZ)	-531.45241	-531.31698	0.1354	2.376
12	GM	8-P2-IS	-1492.263608	-1492.12454	-0.1391	-0.8802
13	TS	8-P2-TS	-1490.862977	-1490.96045	0.09747	0.6169
14	FS(2NN)	8-P2-FS	-1491.151126	-1491.08013	-0.07099	-0.4493
15	GM	10-P3-IS	-1208.739024	-1208.561128	-0.1779	-1.3898
16	TS2	10-P3-TS	-1207.090319	-1207.05292	-0.03739	-0.2922
17	FS(2NN_a)	10-P3-FS	-1207.526638	-1207.37878	-0.1479	-1.1551
*18	Zr4Y2O11	GM(20YSZ)	-160.18734	-160.15011	0.0372	2.19
19	Zr5Y2O13	GM(16.7YSZ)	-188.60247	-188.61846	-0.0159	-0.799
20	Zr6Y2O15	GM(14.3YSZ)	-216.96546	-216.94651	0.019	0.824
-	RMS†	-	-	-	-	1.382

†: Root mean sqaure (RMS) error of energy deviation between DFT and NN PES.

*. 18-20 XYZ coordinates taken from the reported GM in Ref. [6].

We also compared the energy difference of five structures for 8YSZ (including the GM) by empirical potential, G-NN potential and DFT calculations. The empirical potential utilized is that employed in most studies for YZrO system[7, 8-13] , which models the ion-ion interaction via the Buckingham potential[8] and the Coulombic potential. The results are shown in **Table S3.** It is obvious that the energy ordering obtained from empirical potential is not good and the absolute energy error as compared with DFT calculations is also rather large, ~10.5 meV/atom. Instead, our G-NN potential performs well in comparsion with DFT calculations and for the five structures the error is

within 1.7 meV/atom.

Table S3 | Benchmark of empirical potential, G-NN potential calculations for 8YSZ systems (79-atom per cell) as compared with DFT results. The energy is with respect to the GM of 8YSZ calculated by each calculation setup (set as energy zero).

Structure*	E_{emp}/eV	E_{NN}/eV	E_{DFT}/eV	$\Delta E_{emp\text{-}DFT}$ (meV/atom)	$\Delta E_{NN\text{-}DFT}$ (meV/atom)
Str-1	0.4926	0.1034	0.2334	3.281	-1.646
Str-2	0.3330	0.2558	0.2520	1.026	0.0481
Str-3	0.8855	0.3401	0.4330	5.729	-1.176
Str-8	-0.2955	0.4710	0.5300	-10.449	-0.747

*All XYZ coordinates are included in SI part 8.

4. Automated SSW-RS to searh the anion diffusion pathways

In our implementation, the migration mechanism of anion has been investigated using SSW-based reaction sampling (SSW-RS) method to sample exhaustively the possible pathways. In the following, we describe in brief here the SSW-RS method, which can also be found in our previous work[14]. The SSW pathway sampling is fully automated and divided into two stages in simulation, namely,

(i) **Pathway collection via extensive SSW global search**; The reaction sampling is carried out by using the SSW method, which aims to generate an ensemble of reactant–product pairs for pathway building. The structures of the reactant–product pair are geometrically close on PES thanks to the smooth structure perturbation of the SSW method, and they can be utilized later for TS location and pathway determination using the double-ended TS searching method, e.g. double-ended surface walking method (DESW)[15] in this work. The SSW reaction sampling starts from the GM as the intial state (IS) in this work to study the anion diffusion pathway, which is the input structure. During the simulation, the structures nearby this IS will be visited, including the conformation isomers of the same IS (such as the anion diffusion to its 1NN, 2NN and farther positions) and other new phases, defined as the final state (FS).

(ii) **Pathway building and TS determination via DESW** ; Once enough IS/FS pairs are collected, we then need to find the reaction pathways connecting these IS/FS pairs.pathway screening via fast DESW pathway building. The DESW method operates with two structural images starting from the IS and the FS, respectively, to walk step-wisely towards each other. The surface walking involves the repeated bias potential addition and local relaxation with the biased-CBD method to correct the walking direction, in a manner similar to the SSW and BP-CBD method. Since the TS location is the concern, the Gaussian width utilized in the DESW method is generally much smaller, e.g. 0.1–0.2 Å, compared to that (0.6 Å) in the SSW method for PES exploration. The DESW method can fast build a pseudo pathway to connect two minima since the added Gaussian functions effectively smooth the corrugated PES. The TS location is then performed from the highest energy image point at the pseudo pathway using the single-ended CBD TS searching method.

5. Supercells utilized in SSW global optimization and the representative structurs in 8YSZ

Table S4 | Supercells utilized for SSW global optimization for each composition

Formular	N_Zr	N_Y	N_O	N_O$_v$	O$_v$(%)	Total ions	Y$_2$O$_3$(mol%)	YO$_{1.5}$(mol%)
Y2Zr18O39	18	2	39	1	2.564	59	5.3	10.06
Y2Zr14O31	14	2	31	1	3.226	47	6.7	12.56
Y4Zr23O52	23	4	52	2	3.846	79	8	14.81
Y8Zr46O104	46	8	104	4	3.846	158	8	14.81
Y16Zr92O208	92	16	208	8	3.846	316	8	14.81
Y2Zr9O21	9	2	21	1	4.762	32	10	18.18
Y4Zr18O42	18	4	42	2	4.762	64	10	18.18
Y8Zr36O84	36	8	84	4	4.762	128	10	18.18
Y4Zr12O30	12	4	30	2	6.667	46	14.3	25.02
Y4Zr8O22	8	4	22	2	9.091	34	20	33.33
Y8Zr16O44	16	8	44	4	9.091	68	20	33.33
Zr2Y2O7	2	2	7	1	14.286	11	33.3	49.96
Zr4Y4O7	4	4	14	2	14.286	22	33.3	49.96
Zr8Y8O28	8	8	28	4	14.286	44	33.3	49.96
Zr3Y4O12	3	4	12	2	16.667	19	40	57.14
Zr9Y12O36	9	12	36	6	16.667	57	40	57.14
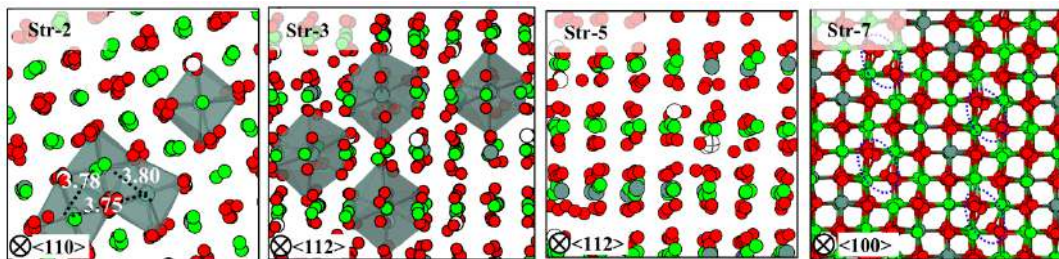
FigureS2. Representative structures (Str-2, Str-3, Str-5 and Str-7 as labeled in Figure 1a). Also see Figure 1a caption for notations.

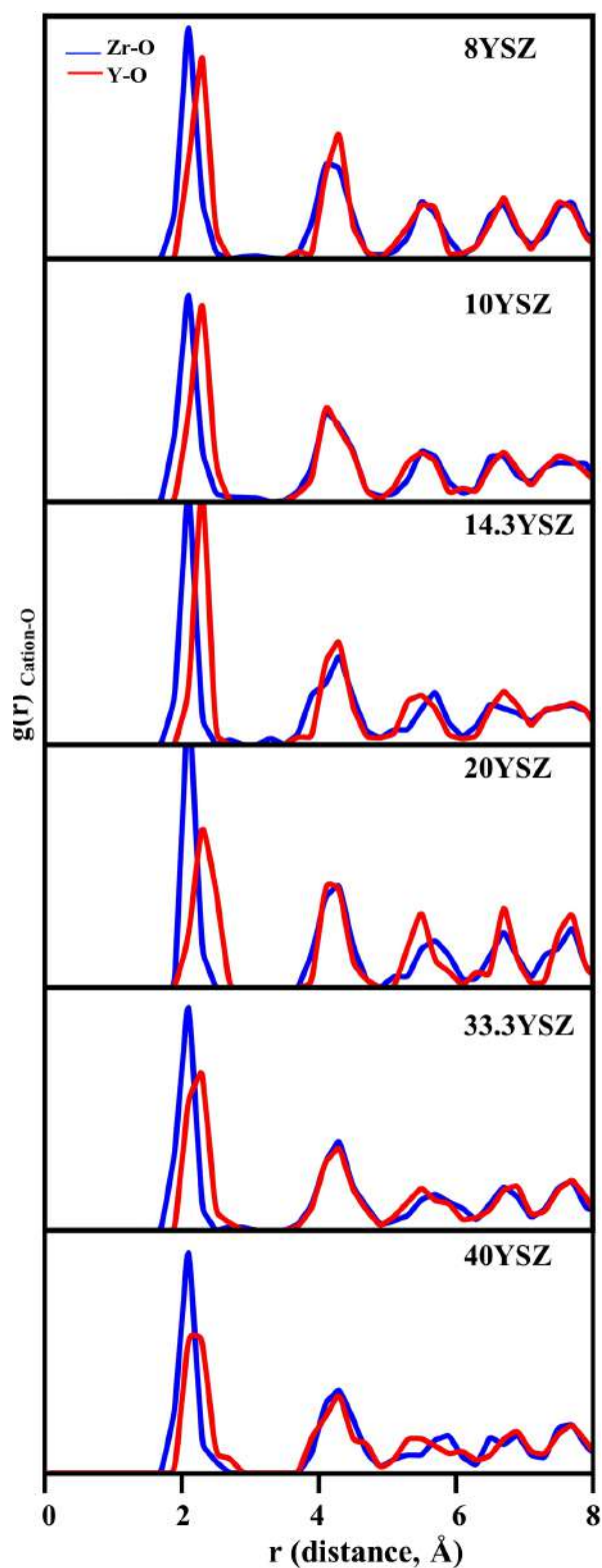**6. RDFs of cation-O pair for GMs of YSZs at different concentrations**

Figure S3 │ Radial distribution function of Cation- O of GMs at different Y concentrations.

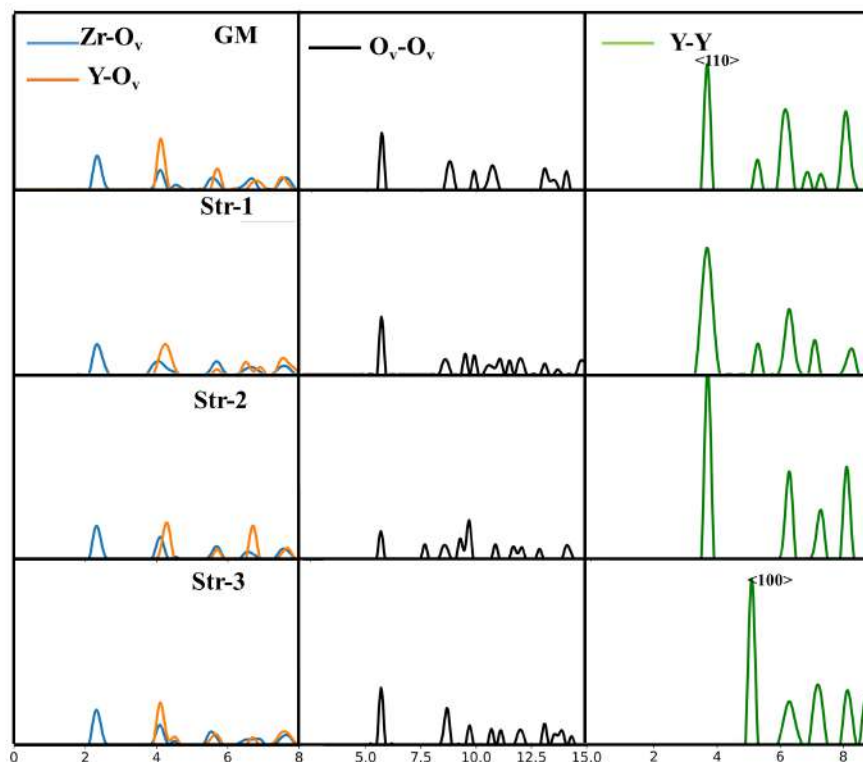## 7. RDF of cation-Ov, Ov-Ov and Y-Y pairs for four low-lying minima in 8YSZ

Figure S4 │ Radial distribution function of GM, Str-1 ,Str-2 and Str-3 structures for 8YSZ.

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8. XYZ coordination of all GM structures and anion diffusion pathway of 8YSZ

GM (6.7YSZ) Energy from NN is -444.369121

!DATE

PBC 15.44811089 5.29330115 7.56017961 96.95827926 102.90582584 95.65305245

O	5.428671190	-0.205981218	4.785950185 CORE	1 O	O	0.0000	1
O	2.693842679	0.055132508	0.202165596 CORE	2 O	O	0.0000	2
O	5.739407878	2.256051926	6.555350718 CORE	3 O	O	0.0000	3
O	13.592022713	-0.333294340	2.799948124 CORE	4 O	O	0.0000	4
O	6.940517711	2.294067278	1.544545032 CORE	5 O	O	0.0000	5
O	0.466279721	0.355466534	1.614935363 CORE	6 O	O	0.0000	6
O	12.165617943	2.400096921	1.535933750 CORE	7 O	O	0.0000	7
O	12.867075883	-0.427107222	6.667724866 CORE	8 O	O	0.0000	8
O	2.899366102	2.887075449	1.748200969 CORE	9 O	O	0.0000	9
O	5.814792466	5.113025094	0.981884206 CORE	10 O	O	0.0000	10
O	7.633088750	1.760216417	4.262485995 CORE	11 O	O	0.0000	11
O	2.260303690	1.871327102	4.092016686 CORE	12 O	O	0.0000	12
O	9.781210972	1.710110020	6.107844511 CORE	13 O	O	0.0000	13
O	3.025329606	1.386441019	6.969115362 CORE	14 O	O	0.0000	14
O	9.696287661	3.145311835	1.024732502 CORE	15 O	O	0.0000	15
O	10.113318895	0.256104358	2.094292539 CORE	16 O	O	0.0000	16
O	14.355623996	2.014791135	3.374582979 CORE	17 O	O	0.0000	17
O	10.353299693	2.750515870	3.782790725 CORE	18 O	O	0.0000	18
O	7.325993996	4.793144416	3.144475480 CORE	19 O	O	0.0000	19
O	5.061841276	2.577285986	3.662227927 CORE	20 O	O	0.0000	20
O	-0.516112762	3.111082818	1.078495320 CORE	21 O	O	0.0000	21
O	12.514525153	2.456606771	5.660896188 CORE	22 O	O	0.0000	22
O	2.766351183	4.167946210	5.947101585 CORE	23 O	O	0.0000	23
O	4.235273932	0.009412872	2.442602800 CORE	24 O	O	0.0000	24
O	12.296866911	0.003347048	0.506928543 CORE	25 O	O	0.0000	25
O	11.563961273	-0.079998468	4.350805691 CORE	26 O	O	0.0000	26
O	7.002055734	-0.488008258	7.126337779 CORE	27 O	O	0.0000	27
O	-0.448880607	-0.737133177	5.045783416 CORE	28 O	O	0.0000	28
O	9.236921178	-0.720755751	5.567312702 CORE	29 O	O	0.0000	29
O	-0.399615878	1.738827346	6.128669855 CORE	30 O	O	0.0000	30
O	1.367580793	4.567904739	3.579802197 CORE	31 O	O	0.0000	31
Y	1.482413445	0.423545077	5.638289980 CORE	32 Y	Y	0.0000	32
Y	6.687796297	3.593841270	5.053353760 CORE	33 Y	Y	0.0000	33
Zr	6.196168523	0.964502150	2.962047864 CORE	34 Zr	Zr	0.0000	34
Zr	-0.540718714	3.946143701	3.017230114 CORE	35 Zr	Zr	0.0000	35
Zr	9.465059879	0.858463620	4.101403330 CORE	36 Zr	Zr	0.0000	36
Zr	11.122649908	4.047630925	2.350172048 CORE	37 Zr	Zr	0.0000	37
Zr	10.668950484	3.556011410	5.776806458 CORE	38 Zr	Zr	0.0000	38
Zr	10.645130035	1.447883071	0.227783772 CORE	39 Zr	Zr	0.0000	39

Zr	13.898862485	1.271664216	1.340183769 CORE	40 Zr	Zr	0.0000	40
Zr	13.472231543	0.798808667	4.881133033 CORE	41 Zr	Zr	0.0000	41
Zr	4.016536737	4.213884485	0.490772240 CORE	42 Zr	Zr	0.0000	42
Zr	-1.445777842	3.342430982	6.909192909 CORE	43 Zr	Zr	0.0000	43
Zr	3.363768076	3.661664953	3.934912214 CORE	44 Zr	Zr	0.0000	44
Zr	4.943883107	0.408147639	6.807023886 CORE	45 Zr	Zr	0.0000	45
Zr	7.876035444	4.152939883	1.190294488 CORE	46 Zr	Zr	0.0000	46
Zr	2.387791716	0.978342163	2.213497784 CORE	47 Zr	Zr	0.0000	47

end
end

GM-1 (6.7YSZ)   Energy from NN is   -443.874952

!DATE
PBC   7.36802144   12.12066432   7.42480381   99.50444057   60.34510283   98.19883856

O	3.607124214	10.528617591	5.373124129 CORE	1 O	O	0.0000	1
O	7.793299790	4.697896232	6.282395704 CORE	2 O	O	0.0000	2
O	3.319989212	6.652172086	3.898852437 CORE	3 O	O	0.0000	3
O	3.878038451	3.926629076	2.066000311 CORE	4 O	O	0.0000	4
O	2.051643103	11.241901989	0.973849471 CORE	5 O	O	0.0000	5
O	5.967019510	3.294484831	5.231856477 CORE	6 O	O	0.0000	6
O	4.058799263	8.331816520	2.335953026 CORE	7 O	O	0.0000	7
O	3.826331878	0.487599540	6.132074631 CORE	8 O	O	0.0000	8
O	2.216835279	6.626362903	1.207606737 CORE	9 O	O	0.0000	9
O	2.266012487	0.481411181	2.881729038 CORE	10 O	O	0.0000	10
O	6.029769490	11.232277950	1.495272976 CORE	11 O	O	0.0000	11
O	6.986771355	3.972800348	1.487847396 CORE	12 O	O	0.0000	12
O	7.738293360	6.785454507	4.592886463 CORE	13 O	O	0.0000	13
O	5.764265950	6.806374950	1.182988096 CORE	14 O	O	0.0000	14
O	7.580175190	11.074619787	4.984734632 CORE	15 O	O	0.0000	15
O	3.989069788	4.847655050	5.872891178 CORE	16 O	O	0.0000	16
O	5.709880084	5.223490475	3.425136007 CORE	17 O	O	0.0000	17
O	5.755770382	9.701760341	3.705760148 CORE	18 O	O	0.0000	18
O	2.016634576	2.499066127	1.025234688 CORE	19 O	O	0.0000	19
O	1.644715494	4.646625891	3.583975760 CORE	20 O	O	0.0000	20
O	7.058234577	0.629242404	5.565610993 CORE	21 O	O	0.0000	21
O	4.131327541	2.003095433	3.934266693 CORE	22 O	O	0.0000	22
O	0.184479914	8.397793131	2.310576839 CORE	23 O	O	0.0000	23
O	7.553789168	1.980841335	3.249930412 CORE	24 O	O	0.0000	24
O	5.664134077	-0.228637427	2.944005643 CORE	25 O	O	0.0000	25
O	5.518673698	7.736423777	5.507583864 CORE	26 O	O	0.0000	26
O	1.994241668	9.593637825	3.657864628 CORE	27 O	O	0.0000	27
O	4.120617145	9.808656556	0.209461550 CORE	28 O	O	0.0000	28
O	5.172646958	1.884605565	1.249538796 CORE	29 O	O	0.0000	29
O	2.701775137	7.873459748	5.955619178 CORE	30 O	O	0.0000	30
O	9.421752206	2.613349851	5.343081013 CORE	31 O	O	0.0000	31

Y	2.185693826	9.022345935	1.351455558 CORE	32 Y	Y	0.0000	32
Y	7.646433782	6.004048089	2.290782564 CORE	33 Y	Y	0.0000	33
Zr	2.090032108	0.392345136	0.640179243 CORE	34 Zr	Zr	0.0000	34
Zr	7.691498018	-0.100910046	3.718916752 CORE	35 Zr	Zr	0.0000	35
Zr	6.004443443	5.565523759	5.491450331 CORE	36 Zr	Zr	0.0000	36
Zr	3.912922361	8.668060762	4.447721680 CORE	37 Zr	Zr	0.0000	37
Zr	4.075905947	6.025857924	2.084911371 CORE	38 Zr	Zr	0.0000	38
Zr	2.229300673	2.742726765	3.186622184 CORE	39 Zr	Zr	0.0000	39
Zr	7.512552771	8.898973895	4.501194234 CORE	40 Zr	Zr	0.0000	40
Zr	3.967496493	3.199695069	0.007361752 CORE	41 Zr	Zr	0.0000	41
Zr	3.934832441	-0.270699946	4.151432698 CORE	42 Zr	Zr	0.0000	42
Zr	9.529543114	5.816257195	5.399058686 CORE	43 Zr	Zr	0.0000	43
Zr	5.757877254	9.055605372	1.449608897 CORE	44 Zr	Zr	0.0000	44
Zr	4.081438105	2.636515625	6.104643052 CORE	45 Zr	Zr	0.0000	45
Zr	5.792737669	-0.017291299	0.757322055 CORE	46 Zr	Zr	0.0000	46
Zr	5.786891466	3.075777296	2.973933734 CORE	47 Zr	Zr	0.0000	47

end
end

GM (8YSZ) Energy from NN is   -746.054580

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PBC   9.90282953   8.90961161   10.95996185   89.59246758   101.69302410   89.12748902

O	9.206573932	7.664044368	0.859154672 CORE	1 O	O	0.0000	1
O	5.624739754	4.754614460	7.520133063 CORE	2 O	O	0.0000	2
Y	-1.195875669	2.590077640	9.676452472 CORE	3 Y	Y	0.0000	3
Y	4.582933121	8.641117077	3.275298443 CORE	4 Y	Y	0.0000	4
Y	2.315597649	5.733342873	2.956951555 CORE	5 Y	Y	0.0000	5
Y	6.489489123	8.669354267	9.296884980 CORE	6 Y	Y	0.0000	6
O	2.393091157	8.092660030	2.861748167 CORE	7 O	O	0.0000	7
O	3.805354159	2.393883266	6.838100701 CORE	8 O	O	0.0000	8
Zr	1.261221747	8.551162190	1.131289013 CORE	9 Zr	Zr	0.0000	9
O	8.002725896	3.472429689	7.540583501 CORE	10 O	O	0.0000	10
Zr	0.027722443	8.512264408	8.063856271 CORE	11 Zr	Zr	0.0000	11
O	2.763946439	0.784308480	8.688906383 CORE	12 O	O	0.0000	12
O	8.676521799	3.287352437	4.213337207 CORE	13 O	O	0.0000	13
Zr	7.958014212	5.596475948	7.691218841 CORE	14 Zr	Zr	0.0000	14
O	2.947335837	6.311303417	10.509960734 CORE	15 O	O	0.0000	15
O	7.006073809	4.913417889	3.209452150 CORE	16 O	O	0.0000	16
Zr	-0.562618712	2.589265002	6.103965662 CORE	17 Zr	Zr	0.0000	17
O	8.199790739	7.575147424	3.882304845 CORE	18 O	O	0.0000	18
O	5.618115437	0.494895772	7.277720452 CORE	19 O	O	0.0000	19
O	0.982048658	1.991294188	4.537442449 CORE	20 O	O	0.0000	20
O	2.967068624	0.477140403	5.162228768 CORE	21 O	O	0.0000	21
Zr	1.186702970	8.721156831	4.640621251 CORE	22 Zr	Zr	0.0000	22
O	-0.023236589	5.017887969	2.519115423 CORE	23 O	O	0.0000	23

O	4.461807953	7.706168494	9.004339938 CORE	24 O	O	0.0000	24
Zr	4.350118054	5.574738701	8.964997937 CORE	25 Zr	Zr	0.0000	25
O	6.403953115	2.164402772	9.210409683 CORE	26 O	O	0.0000	26
O	4.203942377	0.710709094	1.099905191 CORE	27 O	O	0.0000	27
Zr	1.550416138	5.710603678	6.506105566 CORE	28 Zr	Zr	0.0000	28
O	2.977528510	4.880621082	5.095277148 CORE	29 O	O	0.0000	29
O	7.047565361	0.638050228	0.181410220 CORE	30 O	O	0.0000	30
Zr	2.933975452	2.750957364	4.943593975 CORE	31 Zr	Zr	0.0000	31
O	5.487086619	3.676528609	5.174135962 CORE	32 O	O	0.0000	32
O	7.172327104	6.105739112	5.782707738 CORE	33 O	O	0.0000	33
Zr	3.586321661	2.685792366	1.481868185 CORE	34 Zr	Zr	0.0000	34
O	2.165845104	3.480290934	2.907773815 CORE	35 O	O	0.0000	35
O	6.736248553	6.342419673	9.234630409 CORE	36 O	O	0.0000	36
Zr	0.173932272	2.716497603	2.598362443 CORE	37 Zr	Zr	0.0000	37
O	5.298850534	7.880305123	5.334231281 CORE	38 O	O	0.0000	38
O	7.989105495	7.923292344	7.498874449 CORE	39 O	O	0.0000	39
O	3.768932209	6.505027251	6.907770056 CORE	40 O	O	0.0000	40
Zr	8.730186378	5.583380430	4.226723669 CORE	41 Zr	Zr	0.0000	41
O	0.036442436	6.330335684	8.058846718 CORE	42 O	O	0.0000	42
O	6.490533117	0.656154907	3.638289237 CORE	43 O	O	0.0000	43
Zr	7.490397268	2.761174975	0.163440653 CORE	44 Zr	Zr	0.0000	44
O	5.739235135	3.253767322	1.603812690 CORE	45 O	O	0.0000	45
O	1.079704591	3.276399331	10.104179560 CORE	46 O	O	0.0000	46
Zr	3.081099096	8.495411064	10.474239484 CORE	47 Zr	Zr	0.0000	47
O	0.864812339	6.615874144	4.589220491 CORE	48 O	O	0.0000	48
O	7.220569539	1.807023009	5.757481288 CORE	49 O	O	0.0000	49
Zr	3.828735075	8.632792566	7.036550818 CORE	50 Zr	Zr	0.0000	50
O	0.180670234	1.705553235	8.005638309 CORE	51 O	O	0.0000	51
O	-1.370679917	0.259431219	9.809071247 CORE	52 O	O	0.0000	52
Zr	5.059454060	5.731968321	5.447569279 CORE	53 Zr	Zr	0.0000	53
O	8.016144703	2.051103518	2.117089745 CORE	54 O	O	0.0000	54
O	1.612252032	1.729252513	1.155626886 CORE	55 O	O	0.0000	55
Zr	5.690852032	5.482525600	1.711087160 CORE	56 Zr	Zr	0.0000	56
O	-1.101344443	4.864337844	9.724977977 CORE	57 O	O	0.0000	57
O	4.281259754	2.105288709	3.458003264 CORE	58 O	O	0.0000	58
Zr	0.883441919	5.740358469	10.033405545 CORE	59 Zr	Zr	0.0000	59
O	9.512839703	3.359357318	0.581009348 CORE	60 O	O	0.0000	60
O	-0.421522835	4.921476228	6.040390260 CORE	61 O	O	0.0000	61
Zr	9.614989752	5.505458856	0.378014253 CORE	62 Zr	Zr	0.0000	62
O	3.950703805	3.467133339	9.417902174 CORE	63 O	O	0.0000	63
O	3.682908439	4.872321726	1.292408190 CORE	64 O	O	0.0000	64
Zr	7.905061851	8.810297098	2.137972546 CORE	65 Zr	Zr	0.0000	65
O	1.433641302	3.424587019	6.566607242 CORE	66 O	O	0.0000	66
O	-0.597005080	0.362576147	5.833320001 CORE	67 O	O	0.0000	67

O	1.651469897	6.487210485	0.783379235 CORE	68 O	O	0.0000	68
O	4.562801082	6.210471824	3.404821717 CORE	69 O	O	0.0000	69
Zr	7.278138619	8.572051323	5.588233688 CORE	70 Zr	Zr	0.0000	70
O	1.644094915	7.950603725	6.742053078 CORE	71 O	O	0.0000	71
O	6.165631306	7.604610182	1.691743219 CORE	72 O	O	0.0000	72
Zr	5.914230979	2.650185891	7.165124441 CORE	73 Zr	Zr	0.0000	73
O	1.135285102	7.875408787	9.793061398 CORE	74 O	O	0.0000	74
O	2.263433811	5.068245950	8.403320515 CORE	75 O	O	0.0000	75
Zr	6.560478217	2.796637190	3.625426156 CORE	76 Zr	Zr	0.0000	76
O	7.471897879	5.010216181	0.291265861 CORE	77 O	O	0.0000	77
O	-0.055868963	0.434966349	2.735449142 CORE	78 O	O	0.0000	78
Zr	2.220870005	2.778046601	8.390356627 CORE	79 Zr	Zr	0.0000	79

end
end

Str-1 Energy from NN is   -745.951219

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PBC   9.91977936   11.48774887   9.63323289   89.23106676   109.93630623   69.05217678

O	10.003084385	3.279152904	2.286717328 CORE	1 O	O	0.0000	1
O	4.859436767	3.216279302	0.028899757 CORE	2 O	O	0.0000	2
Zr	2.739605587	1.541882648	4.919602210 CORE	3 Zr	Zr	0.0000	3
Zr	2.367990340	7.757834170	5.952339067 CORE	4 Zr	Zr	0.0000	4
O	9.456126926	9.356850795	2.624148051 CORE	5 O	O	0.0000	5
O	0.627603523	1.625291216	4.286851097 CORE	6 O	O	0.0000	6
O	8.214285953	2.192882416	5.280002891 CORE	7 O	O	0.0000	7
Zr	8.445453092	9.032891177	8.900257346 CORE	8 Zr	Zr	0.0000	8
O	4.702144288	6.228289951	2.648978864 CORE	9 O	O	0.0000	9
O	2.800775340	8.220828385	7.975393318 CORE	10 O	O	0.0000	10
Zr	11.112813545	4.266857890	0.591876002 CORE	11 Zr	Zr	0.0000	11
O	7.094923141	6.535113478	5.301234054 CORE	12 O	O	0.0000	12
O	11.742233391	8.631806395	1.885796068 CORE	13 O	O	0.0000	13
Zr	0.527608293	1.140560972	2.142399810 CORE	14 Zr	Zr	0.0000	14
O	8.638585953	1.198226535	1.037710020 CORE	15 O	O	0.0000	15
O	5.570866908	10.614519333	6.062308002 CORE	16 O	O	0.0000	16
O	5.285288696	9.914396492	1.575581400 CORE	17 O	O	0.0000	17
O	3.131550340	10.651248603	3.239619622 CORE	18 O	O	0.0000	18
O	6.965561494	1.448480893	8.137111288 CORE	19 O	O	0.0000	19
O	3.605321545	11.769631248	7.383983588 CORE	20 O	O	0.0000	20
Zr	3.455796445	4.997680500	3.864355497 CORE	21 Zr	Zr	0.0000	21
O	6.487712844	9.586110392	8.523011442 CORE	22 O	O	0.0000	22
O	1.145563024	6.321175015	6.933038716 CORE	23 O	O	0.0000	23
Zr	-1.707504479	2.958810411	7.378383695 CORE	24 Zr	Zr	0.0000	24
O	-0.823301718	7.065178084	8.479592399 CORE	25 O	O	0.0000	25
O	7.809018825	5.176676163	7.417949659 CORE	26 O	O	0.0000	26
Zr	7.395425620	9.698896134	2.377964625 CORE	27 Zr	Zr	0.0000	27

O	6.293032570	3.353238475	6.606203123 CORE	28 O	O	0.0000	28
O	7.688986151	10.206388202	4.604670769 CORE	29 O	O	0.0000	29
Zr	2.165357339	10.344071907	8.501893418 CORE	30 Zr	Zr	0.0000	30
O	6.072894014	2.016282384	2.274920432 CORE	31 O	O	0.0000	31
O	4.111598279	4.070547042	7.829781533 CORE	32 O	O	0.0000	32
Zr	9.513123580	10.118630642	5.701780935 CORE	33 Zr	Zr	0.0000	33
O	10.539537200	11.202551226	4.233081683 CORE	34 O	O	0.0000	34
O	4.109860181	2.783614125	3.732789139 CORE	35 O	O	0.0000	35
O	7.327422486	8.715196511	0.469140271 CORE	36 O	O	0.0000	36
Zr	6.170051502	2.588588487	4.484489833 CORE	37 Zr	Zr	0.0000	37
O	4.713264796	1.536214083	5.820189765 CORE	38 O	O	0.0000	38
O	2.346232642	6.848665421	3.880100111 CORE	39 O	O	0.0000	39
Zr	4.931672699	2.016911883	7.906162555 CORE	40 Zr	Zr	0.0000	40
O	8.195248304	8.517458796	6.571868610 CORE	41 O	O	0.0000	41
O	1.964945987	3.827533558	4.780271139 CORE	42 O	O	0.0000	42
Zr	9.013448966	6.566027263	6.319476542 CORE	43 Zr	Zr	0.0000	43
O	9.119303478	10.600664883	7.682230854 CORE	44 O	O	0.0000	44
O	2.574964477	0.982587294	2.827306740 CORE	45 O	O	0.0000	45
Zr	6.306815282	8.664273475	5.558416732 CORE	46 Zr	Zr	0.0000	46
O	2.995183665	4.247065007	1.856885999 CORE	47 O	O	0.0000	47
O	5.818564936	5.817287768	8.892138401 CORE	48 O	O	0.0000	48
Zr	-0.275160970	3.632623234	4.402290079 CORE	49 Zr	Zr	0.0000	49
O	5.397012381	7.493543554	6.962620627 CORE	50 O	O	0.0000	50
O	1.825800319	9.974924446	6.347898551 CORE	51 O	O	0.0000	51
Zr	5.570757699	5.410969719	6.759713679 CORE	52 Zr	Zr	0.0000	52
O	3.491823057	5.775332590	5.997329071 CORE	53 O	O	0.0000	53
O	4.061236702	0.387701037	0.884118837 CORE	54 O	O	0.0000	54
Zr	2.117862988	4.352729836	6.955650660 CORE	55 Zr	Zr	0.0000	55
O	7.630983782	3.978846469	3.531097711 CORE	56 O	O	0.0000	56
O	10.314035765	8.186844458	5.134155427 CORE	57 O	O	0.0000	57
Zr	3.975491960	2.285754246	1.664898075 CORE	58 Zr	Zr	0.0000	58
O	6.693601459	5.229484860	1.265244679 CORE	59 O	O	0.0000	59
O	9.662536704	5.713289884	4.455620582 CORE	60 O	O	0.0000	60
Zr	6.700983362	5.960754965	3.284986327 CORE	61 Zr	Zr	0.0000	61
O	0.004145623	3.838857817	6.522612604 CORE	62 O	O	0.0000	62
O	3.970589719	7.758829522	0.470777338 CORE	63 O	O	0.0000	63
O	6.185826986	8.280736583	3.503144247 CORE	64 O	O	0.0000	64
O	10.703183885	10.708256620	0.191346377 CORE	65 O	O	0.0000	65
Zr	10.255141702	7.385285661	3.071085253 CORE	66 Zr	Zr	0.0000	66
O	2.311599693	2.208279828	6.886914630 CORE	67 O	O	0.0000	67
O	3.952836080	8.852804655	5.054177088 CORE	68 O	O	0.0000	68
Zr	5.627081860	11.422939068	8.210850936 CORE	69 Zr	Zr	0.0000	69
O	5.393915046	4.707305130	4.633451206 CORE	70 O	O	0.0000	70
O	1.772028403	2.150571788	0.505900377 CORE	71 O	O	0.0000	71

Zr	3.524509491	10.954876281	5.382129687 CORE	72 Zr Zr	0.0000	72
O	10.655132907	6.232668364	1.350646206 CORE	73 O O	0.0000	73
O	8.299297200	7.007254507	2.482819516 CORE	74 O O	0.0000	74
Zr	11.113789326	10.683985366	2.240600444 CORE	75 Zr Zr	0.0000	75
Y	4.639817575	5.531355765	0.354468959 CORE	76 Y Y	0.0000	76
Y	7.704767391	3.261977238	1.254602280 CORE	77 Y Y	0.0000	77
Y	3.931067030	8.381818911	2.762013387 CORE	78 Y Y	0.0000	78
Y	8.197826670	6.611800724	0.163980526 CORE	79 Y Y	0.0000	79

end

end

Str-2   Energy from NN is   -745.798775

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PBC   9.78221434   11.00692864   9.75553865   92.84051697   105.98618340   70.80895446

O	4.037700565	1.477975021	1.014766475 CORE	1 O O	0.0000	1
O	1.401896740	4.716111535	1.288937421 CORE	2 O O	0.0000	2
Y	4.849534523	5.832718161	8.256826124 CORE	3 Y Y	0.0000	3
Y	4.761787836	10.171179979	3.755619897 CORE	4 Y Y	0.0000	4
Y	7.387214158	0.937582702	3.426050921 CORE	5 Y Y	0.0000	5
Y	12.377839680	8.857679727	0.912074421 CORE	6 Y Y	0.0000	6
Zr	5.531082052	2.389494899	9.350715290 CORE	7 Zr Zr	0.0000	7
Zr	3.202915609	1.318461604	6.394884156 CORE	8 Zr Zr	0.0000	8
Zr	-0.293005335	1.952774961	6.268463059 CORE	9 Zr Zr	0.0000	9
O	0.555978800	4.900069643	8.685197259 CORE	10 O O	0.0000	10
O	5.364669565	6.188657928	2.473391143 CORE	11 O O	0.0000	11
Zr	3.929583442	9.016795913	7.125445458 CORE	12 Zr Zr	0.0000	12
O	3.302169742	6.258025218	4.077115729 CORE	13 O O	0.0000	13
Zr	9.581887556	6.393300636	1.712855402 CORE	14 Zr Zr	0.0000	14
O	8.871324779	10.457582279	2.840833070 CORE	15 O O	0.0000	15
O	4.251043666	9.961839801	9.243165129 CORE	16 O O	0.0000	16
Zr	10.144402801	10.491152955	6.963918124 CORE	17 Zr Zr	0.0000	17
O	4.149555680	2.948748677	5.395438791 CORE	18 O O	0.0000	18
O	3.230638518	7.543104726	8.686128334 CORE	19 O O	0.0000	19
Zr	5.490445547	6.808268253	4.484458931 CORE	20 Zr Zr	0.0000	20
O	9.427314305	7.465075612	3.886978993 CORE	21 O O	0.0000	21
O	7.107766505	6.331714829	8.986395711 CORE	22 O O	0.0000	22
O	1.728732457	2.987782547	6.494036506 CORE	23 O O	0.0000	23
O	7.572752078	5.712471962	1.199597648 CORE	24 O O	0.0000	24
Zr	3.829953088	2.141318573	2.981334869 CORE	25 Zr Zr	0.0000	25
O	2.731923407	1.363309896	8.390366946 CORE	26 O O	0.0000	26
O	9.462966638	4.943273207	3.250986377 CORE	27 O O	0.0000	27
Zr	6.194577797	3.521902371	5.708463794 CORE	28 Zr Zr	0.0000	28
O	3.583823361	6.797638053	0.538939529 CORE	29 O O	0.0000	29
O	4.421166877	8.420643930	5.125734516 CORE	30 O O	0.0000	30
O	7.618079678	9.090105142	9.326708121 CORE	31 O O	0.0000	31

O	5.166649363	1.630597081	7.356865429 CORE	32 O	O	0.0000	32
Zr	8.819110434	5.752562244	5.132823677 CORE	33 Zr	Zr	0.0000	33
O	6.904256420	4.949793571	4.284269733 CORE	34 O	O	0.0000	34
O	2.481719734	10.639848565	7.292631313 CORE	35 O	O	0.0000	35
Zr	2.847137827	4.675728966	5.535649373 CORE	36 Zr	Zr	0.0000	36
O	8.186476835	2.820956534	2.107118882 CORE	37 O	O	0.0000	37
O	6.269400416	4.010186896	7.776966098 CORE	38 O	O	0.0000	38
Zr	6.332074656	7.780469211	1.258203950 CORE	39 Zr	Zr	0.0000	39
O	3.235048869	0.633497545	4.356130752 CORE	40 O	O	0.0000	40
O	2.250265064	7.992941034	6.386038812 CORE	41 O	O	0.0000	41
O	4.836777061	9.274261237	1.454422624 CORE	42 O	O	0.0000	42
Zr	1.269108538	6.765017737	7.875217657 CORE	43 Zr	Zr	0.0000	43
O	4.452421968	3.885612900	1.645211849 CORE	44 O	O	0.0000	44
O	6.432295859	8.463615638	3.361175872 CORE	45 O	O	0.0000	45
Zr	6.495128740	4.197077327	2.172003512 CORE	46 Zr	Zr	0.0000	46
O	1.210664066	0.390607489	6.187682822 CORE	47 O	O	0.0000	47
O	2.438063368	3.712240718	3.520720442 CORE	48 O	O	0.0000	48
O	5.843369552	2.662804685	3.518884610 CORE	49 O	O	0.0000	49
O	-0.089127021	1.800678239	4.156284128 CORE	50 O	O	0.0000	50
Zr	3.181221709	5.544099999	2.083024208 CORE	51 Zr	Zr	0.0000	51
O	6.568616875	3.337204513	0.131294509 CORE	52 O	O	0.0000	52
O	-0.208485168	2.522931175	8.321427482 CORE	53 O	O	0.0000	53
Zr	8.924621984	10.069546823	0.749077109 CORE	54 Zr	Zr	0.0000	54
O	1.814893347	1.424145506	2.225597671 CORE	55 O	O	0.0000	55
O	6.868967940	0.691693740	9.071952564 CORE	56 O	O	0.0000	56
Zr	7.684298065	7.987310059	7.604886505 CORE	57 Zr	Zr	0.0000	57
O	7.292004302	0.501684991	1.149790915 CORE	58 O	O	0.0000	58
O	2.573037648	9.486273724	3.264342772 CORE	59 O	O	0.0000	59
Zr	1.708818209	7.898712775	4.364015696 CORE	60 Zr	Zr	0.0000	60
O	11.442423810	7.174321517	2.288286733 CORE	61 O	O	0.0000	61
O	5.610657473	7.907087086	7.522888988 CORE	62 O	O	0.0000	62
Zr	0.495232701	3.136206885	2.528179362 CORE	63 Zr	Zr	0.0000	63
O	8.953823956	6.358107264	7.239424504 CORE	64 O	O	0.0000	64
O	10.249137495	9.615475815	5.008106120 CORE	65 O	O	0.0000	65
Zr	8.291687208	4.582940791	8.501833942 CORE	66 Zr	Zr	0.0000	66
O	2.785885912	5.161159935	7.565873060 CORE	67 O	O	0.0000	67
O	7.909595916	9.782370379	6.362561531 CORE	68 O	O	0.0000	68
O	9.855294259	8.670821239	7.908263674 CORE	69 O	O	0.0000	69
O	4.891746980	5.385654674	5.941426437 CORE	70 O	O	0.0000	70
O	10.154979848	2.610561523	0.467973435 CORE	71 O	O	0.0000	71
O	7.368040661	7.305482095	5.477906415 CORE	72 O	O	0.0000	72
Zr	1.874470286	3.314904067	8.777430991 CORE	73 Zr	Zr	0.0000	73
O	8.500115466	3.968905371	6.272393101 CORE	74 O	O	0.0000	74
O	1.097349332	5.878681872	5.536262817 CORE	75 O	O	0.0000	75

Zr	8.179310909	9.162416544	4.338152562 CORE	76 Zr Zr	0.0000	76
O	7.328131923	1.740864633	5.672562893 CORE	77 O O	0.0000	77
O	8.357775966	8.122938845	1.506631488 CORE	78 O O	0.0000	78
Zr	1.815743292	0.593840005	0.272565607 CORE	79 Zr Zr	0.0000	79

end
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Str-3   Energy from NN is   -745.714432

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PBC   9.82985650   8.82031376   11.10605064   91.05837522   99.13652525   89.91935333

O	8.013631814	5.244261911	0.493809388 CORE	1 O O	0.0000	1
O	2.007157392	8.086142082	10.479034777 CORE	2 O O	0.0000	2
Y	7.466585548	-0.059665906	9.718515753 CORE	3 Y Y	0.0000	3
Y	0.364758990	2.823130184	6.408973494 CORE	4 Y Y	0.0000	4
Y	5.969683616	5.848304954	5.567632745 CORE	5 Y Y	0.0000	5
Y	1.899425828	5.788715992	10.324977375 CORE	6 Y Y	0.0000	6
Zr	3.159995051	6.056101946	3.265069009 CORE	7 Zr Zr	0.0000	7
Zr	0.929482010	2.886105532	2.859002143 CORE	8 Zr Zr	0.0000	8
Zr	5.411342937	5.631933821	9.532414955 CORE	9 Zr Zr	0.0000	9
O	8.234377145	6.432327552	6.076872734 CORE	10 O O	0.0000	10
O	3.805189061	0.603802376	5.431743746 CORE	11 O O	0.0000	11
Zr	0.221400951	6.034416925	0.563811445 CORE	12 Zr Zr	0.0000	12
O	8.507108549	3.866375265	7.585499905 CORE	13 O O	0.0000	13
Zr	-0.736292616	5.839259028	7.960949011 CORE	14 Zr Zr	0.0000	14
O	0.724819408	0.464939662	6.521049057 CORE	15 O O	0.0000	15
O	3.657016281	1.636960956	10.634975042 CORE	16 O O	0.0000	16
Zr	6.667910914	3.006355963	7.862336520 CORE	17 Zr Zr	0.0000	17
O	3.402353521	4.980219495	8.713625109 CORE	18 O O	0.0000	18
O	4.646061759	2.284289964	3.525573881 CORE	19 O O	0.0000	19
Zr	8.193757343	8.676612287	6.194646259 CORE	20 Zr Zr	0.0000	20
O	2.032488549	3.540891023	10.607201218 CORE	21 O O	0.0000	21
O	5.203488813	6.802053422	3.521857042 CORE	22 O O	0.0000	22
O	1.283727099	6.684518069	8.252458188 CORE	23 O O	0.0000	23
O	8.863295391	2.183847253	2.383775221 CORE	24 O O	0.0000	24
Zr	-0.188259140	5.835810350	4.449011041 CORE	25 Zr Zr	0.0000	25
O	0.218364001	8.149866272	0.709516077 CORE	26 O O	0.0000	26
O	1.871828529	2.232583955	4.624359613 CORE	27 O O	0.0000	27
Zr	3.202330880	2.754190574	8.875663234 CORE	28 Zr Zr	0.0000	28
O	-0.532572148	8.223370472	4.418650601 CORE	29 O O	0.0000	29
O	5.212424409	7.843638818	9.271084454 CORE	30 O O	0.0000	30
O	8.273067458	1.820768178	5.679195458 CORE	31 O O	0.0000	31
O	2.555906404	3.463524089	6.885159499 CORE	32 O O	0.0000	32
Zr	1.622932189	0.075453971	4.657373365 CORE	33 Zr Zr	0.0000	33
O	6.753529252	0.786537731	7.723264837 CORE	34 O O	0.0000	34
O	4.709043636	2.253661716	7.361832602 CORE	35 O O	0.0000	35

Zr	2.384061539	8.755502480	1.168726525 CORE	36 Zr Zr	0.0000	36
O	2.326605151	6.630444304	1.214448975 CORE	37 O O	0.0000	37
O	-0.465593433	3.727853692	4.354015808 CORE	38 O O	0.0000	38
Zr	8.723810763	8.742447181	2.387816103 CORE	39 Zr Zr	0.0000	39
O	7.311200677	5.106775117	3.793913916 CORE	40 O O	0.0000	40
O	7.000237020	0.881234547	3.445853314 CORE	41 O O	0.0000	41
O	0.996629130	2.260050859	8.628287745 CORE	42 O O	0.0000	42
Zr	7.442614857	2.891072555	4.026119068 CORE	43 Zr Zr	0.0000	43
O	4.666050244	0.505934312	1.688027825 CORE	44 O O	0.0000	44
O	0.369833667	3.864809416	0.954325182 CORE	45 O O	0.0000	45
Zr	5.973050814	8.651139449	0.152924150 CORE	46 Zr Zr	0.0000	46
O	5.368848604	3.416951179	9.606909442 CORE	47 O O	0.0000	47
O	4.390851996	4.831221542	2.043895825 CORE	48 O O	0.0000	48
O	7.499592067	6.356890050	9.616724568 CORE	49 O O	0.0000	49
O	7.061448772	7.674192936	1.737429142 CORE	50 O O	0.0000	50
Zr	2.603012522	5.603500245	6.805867236 CORE	51 Zr Zr	0.0000	51
O	0.587197781	5.097893546	6.402534668 CORE	52 O O	0.0000	52
O	9.419402452	6.521648869	2.517895980 CORE	53 O O	0.0000	53
Zr	3.983237374	2.814470869	5.431735556 CORE	54 Zr Zr	0.0000	54
O	-0.108757495	0.656542290	10.284643610 CORE	55 O O	0.0000	55
O	6.207298431	8.219194397	5.617825245 CORE	56 O O	0.0000	56
Zr	4.609506625	2.727285343	1.410815621 CORE	57 Zr Zr	0.0000	57
O	5.703339587	6.440406610	0.072202315 CORE	58 O O	0.0000	58
O	3.077201860	8.200901920	3.199779525 CORE	59 O O	0.0000	59
Zr	-0.004606208	2.811283747	10.406388407 CORE	60 Zr Zr	0.0000	60
O	7.820790967	0.934611796	0.392224811 CORE	61 O O	0.0000	61
O	2.477976717	2.269924138	1.373994076 CORE	62 O O	0.0000	62
Zr	8.227414353	3.041843474	0.444379209 CORE	63 Zr Zr	0.0000	63
O	6.084056633	5.049260698	7.684533640 CORE	64 O O	0.0000	64
O	-0.913340164	8.042835261	8.085508095 CORE	65 O O	0.0000	65
Zr	6.360296413	5.661971736	2.032861156 CORE	66 Zr Zr	0.0000	66
O	1.557250046	4.797415788	3.311745837 CORE	67 O O	0.0000	67
O	3.024230548	0.619154440	8.237486978 CORE	68 O O	0.0000	68
O	0.962242767	0.634858489	2.735184838 CORE	69 O O	0.0000	69
O	6.093825621	3.392855948	5.564005066 CORE	70 O O	0.0000	70
O	4.150279711	6.945728702	6.787563816 CORE	71 O O	0.0000	71
O	7.742775186	2.356358688	9.735215601 CORE	72 O O	0.0000	72
Zr	4.794855234	-0.002600731	7.298262564 CORE	73 Zr Zr	0.0000	73
O	3.795617268	4.912408691	5.052495617 CORE	74 O O	0.0000	74
O	-0.200097851	4.936109592	9.909157480 CORE	75 O O	0.0000	75
Zr	5.105908696	0.114946966	3.779905113 CORE	76 Zr Zr	0.0000	76
O	1.770983019	6.813450990	4.959026832 CORE	77 O O	0.0000	77
O	6.595926015	3.441182812	1.792288629 CORE	78 O O	0.0000	78
Zr	1.092878251	0.024237130	8.628387770 CORE	79 Zr Zr	0.0000	79

end

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Str-8   Energy from NN is   -745.557885

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PBC   6.32875872   13.37167394   11.62449004   100.51339312   100.83516901   84.53475805

O	6.319436509	7.603068886	2.750647682 CORE	1 O	O	0.0000	1
O	5.166654103	-0.041372677	1.223848291 CORE	2 O	O	0.0000	2
O	2.663625742	8.987846838	10.010972413 CORE	3 O	O	0.0000	3
O	-0.119597928	1.625442859	4.389983356 CORE	4 O	O	0.0000	4
O	3.915225892	2.118923748	0.484816675 CORE	5 O	O	0.0000	5
O	1.642128116	3.396907700	5.222378114 CORE	6 O	O	0.0000	6
O	-0.131697253	0.195468302	7.385965217 CORE	7 O	O	0.0000	7
O	-0.125703220	5.751456446	6.393589084 CORE	8 O	O	0.0000	8
O	2.179465485	5.862443227	10.136025395 CORE	9 O	O	0.0000	9
O	2.066169270	11.301273276	8.745166059 CORE	10 O	O	0.0000	10
O	-0.001456970	9.979292857	8.084797384 CORE	11 O	O	0.0000	11
O	1.842899015	7.444663837	6.862414453 CORE	12 O	O	0.0000	12
O	2.688257757	0.902037253	5.893222790 CORE	13 O	O	0.0000	13
Zr	-0.301543027	7.991278694	7.165072747 CORE	14 Zr	Zr	0.0000	14
Zr	1.877606773	5.495234926	5.766116713 CORE	15 Zr	Zr	0.0000	15
Zr	4.457008068	12.314449707	5.039985955 CORE	16 Zr	Zr	0.0000	16
Zr	-0.213431766	6.333397412	10.465311708 CORE	17 Zr	Zr	0.0000	17
Zr	5.061237612	5.993933086	4.275260085 CORE	18 Zr	Zr	0.0000	18
Zr	3.106317334	10.598379466	2.243231823 CORE	19 Zr	Zr	0.0000	19
Zr	0.942972007	11.393052833	6.829054567 CORE	20 Zr	Zr	0.0000	20
O	0.848354605	6.771370796	0.383531690 CORE	21 O	O	0.0000	21
O	2.161177921	10.607069122	0.369273680 CORE	22 O	O	0.0000	22
O	3.004381188	7.948466697	0.989900855 CORE	23 O	O	0.0000	23
O	2.901800191	-0.465460265	9.396649503 CORE	24 O	O	0.0000	24
O	-1.362920687	0.944471187	9.984242192 CORE	25 O	O	0.0000	25
O	6.124989223	3.394946676	1.038221997 CORE	26 O	O	0.0000	26
O	4.940162519	9.592399342	1.759694270 CORE	27 O	O	0.0000	27
O	4.143031493	6.145835267	2.384708325 CORE	28 O	O	0.0000	28
O	4.016245379	8.938933934	7.526453864 CORE	29 O	O	0.0000	29
O	4.285728399	7.182852852	11.008498027 CORE	30 O	O	0.0000	30
O	0.580533214	7.753381281	9.115798540 CORE	31 O	O	0.0000	31
O	4.686415750	6.609347132	8.336738462 CORE	32 O	O	0.0000	32
O	3.940503752	-1.189762032	7.080549112 CORE	33 O	O	0.0000	33
O	0.754048155	9.562874590	5.654745431 CORE	34 O	O	0.0000	34
O	2.950028026	11.225713994	6.229400914 CORE	35 O	O	0.0000	35
O	5.167346913	7.898384152	5.174504202 CORE	36 O	O	0.0000	36
O	4.250072875	12.019395673	1.057065863 CORE	37 O	O	0.0000	37
O	3.892011126	0.406137494	3.499698258 CORE	38 O	O	0.0000	38
O	4.014563620	3.258116179	9.112147344 CORE	39 O	O	0.0000	39

O	0.702742457	11.067944852	2.495703190 CORE	40 O	O	0.0000	40
O	2.875204607	12.366008002	3.419646744 CORE	41 O	O	0.0000	41
O	4.942681092	10.380678021	10.194152864 CORE	42 O	O	0.0000	42
O	2.850089031	6.807260866	4.462383059 CORE	43 O	O	0.0000	43
O	0.763655718	5.424206040	3.891208725 CORE	44 O	O	0.0000	44
O	0.701977897	2.438679657	10.672783440 CORE	45 O	O	0.0000	45
O	-0.013954417	4.649817161	9.158978282 CORE	46 O	O	0.0000	46
O	1.912997464	4.814482935	1.748713633 CORE	47 O	O	0.0000	47
O	5.215875759	2.692293507	6.751831396 CORE	48 O	O	0.0000	48
O	0.854446057	1.319211635	2.034255432 CORE	49 O	O	0.0000	49
O	2.596626076	4.961971445	7.717600689 CORE	50 O	O	0.0000	50
O	-0.511741077	-1.371064387	10.966760118 CORE	51 O	O	0.0000	51
O	4.997388998	5.519358739	0.108206983 CORE	52 O	O	0.0000	52
O	1.750165567	2.059758450	8.193875869 CORE	53 O	O	0.0000	53
O	2.122151737	9.033138697	3.295139359 CORE	54 O	O	0.0000	54
O	3.953418081	4.750095145	5.552988162 CORE	55 O	O	0.0000	55
O	6.582956180	12.166131379	4.945953443 CORE	56 O	O	0.0000	56
O	5.097394327	3.917165486	3.303411096 CORE	57 O	O	0.0000	57
O	2.833563365	2.719763169	2.768554495 CORE	58 O	O	0.0000	58
O	4.460748308	10.384549429	4.162894922 CORE	59 O	O	0.0000	59
Zr	6.203856374	11.100057778	0.475058307 CORE	60 Zr	Zr	0.0000	60
Zr	-0.353471468	-0.156884411	3.164165287 CORE	61 Zr	Zr	0.0000	61
Zr	4.097781226	10.887184817	8.341128982 CORE	62 Zr	Zr	0.0000	62
Zr	0.782428624	9.966175398	10.116262151 CORE	63 Zr	Zr	0.0000	63
Zr	4.732744906	4.625291278	7.601314432 CORE	64 Zr	Zr	0.0000	64
Zr	2.761499558	7.348152854	8.759259081 CORE	65 Zr	Zr	0.0000	65
Zr	2.884751544	0.727819010	1.665195233 CORE	66 Zr	Zr	0.0000	66
Zr	0.774921097	1.768754882	6.338970291 CORE	67 Zr	Zr	0.0000	67
Zr	5.185174820	7.649467427	0.868393448 CORE	68 Zr	Zr	0.0000	68
Zr	3.950273383	4.133262302	1.420856743 CORE	69 Zr	Zr	0.0000	69
Zr	6.084832482	1.481671752	0.047670161 CORE	70 Zr	Zr	0.0000	70
Zr	1.917228006	3.779177896	9.455234374 CORE	71 Zr	Zr	0.0000	71
Zr	6.306860635	9.461847327	3.682495580 CORE	72 Zr	Zr	0.0000	72
Zr	-1.372847163	2.837023502	11.017947272 CORE	73 Zr	Zr	0.0000	73
Zr	0.813378853	3.314470137	3.118000837 CORE	74 Zr	Zr	0.0000	74
Zr	2.012536510	6.848131732	2.490846868 CORE	75 Zr	Zr	0.0000	75
Y	0.739861397	0.227109971	9.603279675 CORE	76 Y	Y	0.0000	76
Y	3.943113258	1.050466045	7.974425241 CORE	77 Y	Y	0.0000	77
Y	3.032478661	8.932138455	5.423547927 CORE	78 Y	Y	0.0000	78
Y	3.967503444	2.536703173	4.695746242 CORE	79 Y	Y	0.0000	79

end

end

GM (10YSZ) Energy from NN is   -604.246797

!DATE

PBC	6.35800560	17.41061170	7.41043335	92.23677091	71.65178501	90.00447082
Y	5.259277389	5.277923411	1.220198572 CORE	1 Y	Y	0.0000	1
Y	3.983776787	12.949649370	3.497487457 CORE	2 Y	Y	0.0000	2
Y	7.439144079	8.197656145	6.235098605 CORE	3 Y	Y	0.0000	3
Y	0.813505413	0.454394112	0.552137208 CORE	4 Y	Y	0.0000	4
O	2.474172626	13.980491899	2.010849227 CORE	5 O	O	0.0000	5
O	7.046171180	1.662469754	2.504191083 CORE	6 O	O	0.0000	6
O	1.004636236	4.733578877	0.374567216 CORE	7 O	O	0.0000	7
O	5.071933058	9.479520618	1.465742812 CORE	8 O	O	0.0000	8
Zr	2.583738442	13.223702272	0.036993648 CORE	9 Zr	Zr	0.0000	9
Zr	1.996380799	3.561587667	2.122105909 CORE	10 Zr	Zr	0.0000	10
O	6.141919800	15.901221068	0.919455928 CORE	11 O	O	0.0000	11
O	2.228516141	1.562621355	6.012321532 CORE	12 O	O	0.0000	12
O	2.804874261	16.442075572	5.402768969 CORE	13 O	O	0.0000	13
O	6.041916527	9.340867978	4.477306208 CORE	14 O	O	0.0000	14
O	4.154225252	14.227700685	5.524105955 CORE	15 O	O	0.0000	15
O	8.173635483	10.431104747	6.067926302 CORE	16 O	O	0.0000	16
O	7.300923564	3.741068655	6.228426239 CORE	17 O	O	0.0000	17
O	4.807369302	0.771219775	1.042780289 CORE	18 O	O	0.0000	18
Zr	2.169638952	6.719916342	0.296264805 CORE	19 Zr	Zr	0.0000	19
Zr	1.950262318	0.432618194	4.057755852 CORE	20 Zr	Zr	0.0000	20
O	6.517663806	6.202996909	6.685174029 CORE	21 O	O	0.0000	21
O	6.479550927	4.263762899	2.872849364 CORE	22 O	O	0.0000	22
Zr	6.527407951	8.230564698	2.672888300 CORE	23 Zr	Zr	0.0000	23
Zr	8.325252428	14.567386505	5.982133809 CORE	24 Zr	Zr	0.0000	24
O	5.147376452	3.029292940	4.890959891 CORE	25 O	O	0.0000	25
O	5.082866652	16.641186856	6.900932537 CORE	26 O	O	0.0000	26
O	4.426037450	5.664488233	5.292863607 CORE	27 O	O	0.0000	27
O	2.912554527	2.255374403	3.614182540 CORE	28 O	O	0.0000	28
Zr	3.186155539	3.379258808	5.635123736 CORE	29 Zr	Zr	0.0000	29
Zr	3.938959611	16.245848598	1.468568869 CORE	30 Zr	Zr	0.0000	30
O	4.059720664	11.932941564	1.223896244 CORE	31 O	O	0.0000	31
O	2.294105547	4.657264315	4.237127048 CORE	32 O	O	0.0000	32
O	4.159615964	14.608128858	0.007533113 CORE	33 O	O	0.0000	33
O	1.938790719	16.571207851	2.405462844 CORE	34 O	O	0.0000	34
O	0.978102582	10.283925215	2.443414684 CORE	35 O	O	0.0000	35
O	7.305376048	6.885065133	4.202546874 CORE	36 O	O	0.0000	36
O	2.895902310	5.500435513	1.850110176 CORE	37 O	O	0.0000	37
O	4.234290811	0.050698816	3.439022818 CORE	38 O	O	0.0000	38
Zr	6.429664263	5.017700466	4.813214950 CORE	39 Zr	Zr	0.0000	39
Zr	4.210321030	9.872398751	5.414416495 CORE	40 Zr	Zr	0.0000	40
O	6.229907133	12.608147773	2.865708461 CORE	41 O	O	0.0000	41
O	2.162063424	2.383662706	0.327738827 CORE	42 O	O	0.0000	42
O	3.300277728	10.693470889	3.664578402 CORE	43 O	O	0.0000	43

O	6.374766945	0.548242070	4.924341633 CORE	44 O	O	0.0000	44
Zr	5.018450231	16.126249562	4.895939148 CORE	45 Zr	Zr	0.0000	45
Zr	5.053251549	1.953659716	3.032555835 CORE	46 Zr	Zr	0.0000	46
O	6.915684826	15.271267631	4.455990869 CORE	47 O	O	0.0000	47
O	5.190505901	8.548139283	6.878878464 CORE	48 O	O	0.0000	48
O	0.422933100	13.395427622	0.429041294 CORE	49 O	O	0.0000	49
O	1.780444178	11.164156586	0.271838155 CORE	50 O	O	0.0000	50
Zr	7.230519587	11.262730153	4.340309890 CORE	51 Zr	Zr	0.0000	51
Zr	6.930248649	14.664254838	2.411819085 CORE	52 Zr	Zr	0.0000	52
O	1.974526303	12.942231573	4.672718449 CORE	53 O	O	0.0000	53
O	5.423964826	11.791826364	5.281692735 CORE	54 O	O	0.0000	54
O	2.317988209	8.032276290	2.268072916 CORE	55 O	O	0.0000	55
O	6.588982362	7.337221211	0.720800711 CORE	56 O	O	0.0000	56
Zr	6.103958201	11.420143834	1.062114494 CORE	57 Zr	Zr	0.0000	57
Zr	3.108269927	6.573629550	3.763495527 CORE	58 Zr	Zr	0.0000	58
O	4.811867167	14.982847460	2.976385466 CORE	59 O	O	0.0000	59
O	4.252975948	3.245634396	1.634143631 CORE	60 O	O	0.0000	60
O	4.962495824	6.879251178	2.871251956 CORE	61 O	O	0.0000	61
O	3.121473647	8.163671569	5.119022502 CORE	62 O	O	0.0000	62
Zr	6.439942645	1.864496375	6.628282423 CORE	63 Zr	Zr	0.0000	63
Zr	3.017595691	10.017184488	1.644870755 CORE	64 Zr	Zr	0.0000	64

end

end

GM (14.3YSZ) Energy from NN is   -433.863222

!DATE

PBC 7.36345377 6.35537857 13.05812535 100.32655623 88.66929683 72.05037119

O	8.730094033	3.193189903	4.015173076 CORE	1 O	O	0.0000	1
O	3.348672636	0.569026551	2.023961535 CORE	2 O	O	0.0000	2
O	3.697327833	-0.409640168	8.450807351 CORE	3 O	O	0.0000	3
O	6.973075207	5.075927738	3.249263379 CORE	4 O	O	0.0000	4
O	5.820020822	1.386320415	8.503126381 CORE	5 O	O	0.0000	5
O	3.363320146	1.517806751	4.540958391 CORE	6 O	O	0.0000	6
O	1.682904551	-1.065450671	11.774486629 CORE	7 O	O	0.0000	7
O	5.659954189	-1.154928911	11.693610905 CORE	8 O	O	0.0000	8
O	7.313346584	3.743552594	9.198150566 CORE	9 O	O	0.0000	9
O	1.319433704	0.254208157	5.543473264 CORE	10 O	O	0.0000	10
O	5.322700253	0.177371485	5.744978371 CORE	11 O	O	0.0000	11
O	7.344817402	-0.653948790	8.763524500 CORE	12 O	O	0.0000	12
O	3.584864680	4.184599161	0.669765159 CORE	13 O	O	0.0000	13
O	3.686775848	2.613126535	7.059025617 CORE	14 O	O	0.0000	14
O	5.437206788	3.156305786	3.896222693 CORE	15 O	O	0.0000	15
O	5.355563915	2.252808763	1.447848807 CORE	16 O	O	0.0000	16
O	5.291665850	4.574350900	6.179705333 CORE	17 O	O	0.0000	17
O	1.586154245	1.307491270	7.884150164 CORE	18 O	O	0.0000	18

O	8.938487608	4.330097485	6.492529868 CORE	19 O	O	0.0000	19
O	1.907497236	2.402515086	10.402546962 CORE	20 O	O	0.0000	20
O	6.816473311	2.534172678	6.439074138 CORE	21 O	O	0.0000	21
O	8.981234908	5.911509998	0.117818876 CORE	22 O	O	0.0000	22
O	1.380018918	2.294424422	1.472040775 CORE	23 O	O	0.0000	23
O	6.974645944	4.227405452	0.693510923 CORE	24 O	O	0.0000	24
O	3.953350048	3.665419063	9.400190741 CORE	25 O	O	0.0000	25
O	3.905374736	0.728512558	10.927376830 CORE	26 O	O	0.0000	26
O	5.605638097	3.244523469	11.859692471 CORE	27 O	O	0.0000	27
O	3.586936598	4.987022496	3.168054710 CORE	28 O	O	0.0000	28
O	7.027772411	0.676534975	3.085715858 CORE	29 O	O	0.0000	29
O	7.195295598	0.765210088	11.046183462 CORE	30 O	O	0.0000	30
Y	3.375107465	1.922311095	0.104971323 CORE	31 Y	Y	0.0000	31
Y	1.867722745	0.075971527	9.828621064 CORE	32 Y	Y	0.0000	32
Y	3.404844783	3.844714631	5.114301200 CORE	33 Y	Y	0.0000	33
Y	8.954652864	4.557400556	2.036750969 CORE	34 Y	Y	0.0000	34
Zr	2.092862140	3.310136353	8.427365891 CORE	35 Zr	Zr	0.0000	35
Zr	7.573662275	2.749811806	11.663937032 CORE	36 Zr	Zr	0.0000	36
Zr	5.059927053	1.171595887	3.278970181 CORE	37 Zr	Zr	0.0000	37
Zr	7.042395748	2.138799207	0.025378848 CORE	38 Zr	Zr	0.0000	38
Zr	3.180040938	0.610305671	6.516046643 CORE	39 Zr	Zr	0.0000	39
Zr	5.556174615	3.406886330	8.017220761 CORE	40 Zr	Zr	0.0000	40
Zr	7.207421240	4.134739741	5.178648186 CORE	41 Zr	Zr	0.0000	41
Zr	5.428667679	-0.213466078	9.764629653 CORE	42 Zr	Zr	0.0000	42
Zr	3.635386319	2.762026434	11.662710977 CORE	43 Zr	Zr	0.0000	43
Zr	7.080163164	0.513546993	6.925677404 CORE	44 Zr	Zr	0.0000	44
Zr	5.287526562	4.341544025	2.115990230 CORE	45 Zr	Zr	0.0000	45
Zr	1.634786441	1.158964525	3.280741540 CORE	46 Zr	Zr	0.0000	46

end
end

GM (20YSZ) Energy from NN is   -320.294985

!DATE

PBC   6.41109130   6.38161092   11.07331099   90.27799591   73.39149866   99.51885774

O	4.714527181	0.753263614	9.922475446 CORE	1 O	O	0.0000	1
O	4.611096536	3.080888479	6.292110391 CORE	2 O	O	0.0000	2
O	0.774365947	4.679499861	3.157898867 CORE	3 O	O	0.0000	3
O	1.856362193	1.218788382	4.692025823 CORE	4 O	O	0.0000	4
O	1.559629402	3.452105506	1.056597337 CORE	5 O	O	0.0000	5
O	7.017256307	2.150218279	7.099587019 CORE	6 O	O	0.0000	6
O	2.508309601	5.987627582	0.989999673 CORE	7 O	O	0.0000	7
O	4.637980216	5.795385846	7.748693580 CORE	8 O	O	0.0000	8
O	0.731054129	1.084281617	1.626760442 CORE	9 O	O	0.0000	9
O	1.780061598	4.469781817	6.925137624 CORE	10 O	O	0.0000	10
O	3.521399280	6.087155131	3.954681838 CORE	11 O	O	0.0000	11

O	3.589255839	2.407707609	2.455171929 CORE	12 O	O	0.0000	12
O	4.970061338	1.850260944	0.224235838 CORE	13 O	O	0.0000	13
O	6.023055621	5.232329592	5.517943013 CORE	14 O	O	0.0000	14
O	3.662543439	0.543728625	6.359198099 CORE	15 O	O	0.0000	15
O	4.912823984	5.059062193	1.801170138 CORE	16 O	O	0.0000	16
O	5.970808134	2.164283410	3.694284533 CORE	17 O	O	0.0000	17
O	2.603737729	3.661559496	4.621148167 CORE	18 O	O	0.0000	18
O	2.878828242	1.772871581	8.461982002 CORE	19 O	O	0.0000	19
O	7.019460896	5.553311947	8.990135657 CORE	20 O	O	0.0000	20
O	5.628919426	3.181599921	9.252255791 CORE	21 O	O	0.0000	21
O	2.906939164	4.605867583	9.995782514 CORE	22 O	O	0.0000	22
Zr	3.754650959	2.627040996	10.262833879 CORE	23 Zr	Zr	0.0000	23
Zr	6.047183581	4.189057841	7.437266400 CORE	24 Zr	Zr	0.0000	24
Zr	2.613144734	2.417498080	6.376164579 CORE	25 Zr	Zr	0.0000	25
Zr	2.611607072	6.024870523	8.351272445 CORE	26 Zr	Zr	0.0000	26
Zr	1.562383791	2.636806767	3.049651184 CORE	27 Zr	Zr	0.0000	27
Zr	1.643993704	5.535028300	4.963658677 CORE	28 Zr	Zr	0.0000	28
Zr	4.999344393	0.803405408	2.140470970 CORE	29 Zr	Zr	0.0000	29
Zr	0.509824855	5.325342653	1.074552385 CORE	30 Zr	Zr	0.0000	30
Y	4.787480825	4.052029228	3.913317374 CORE	31 Y	Y	0.0000	31
Y	5.841310968	0.906500994	5.662079970 CORE	32 Y	Y	0.0000	32
Y	3.736824819	3.823171103	0.355126755 CORE	33 Y	Y	0.0000	33
Y	6.897937090	1.150801949	9.216120517 CORE	34 Y	Y	0.0000	34

end

end

GM (33.3YSZ) Energy from NN is   -411.581107

!DATE

PBC   8.52253279   11.82970024   6.48642022   91.15824914   104.11907157   70.94079529

O	2.814481598	2.331315917	0.506091113 CORE	1 O	O	0.0000	1
O	4.631622985	3.412800698	3.995059508 CORE	2 O	O	0.0000	2
O	7.564281657	3.589789282	1.016770405 CORE	3 O	O	0.0000	3
O	7.213361095	2.235822605	3.352531929 CORE	4 O	O	0.0000	4
O	8.040657695	4.456591407	4.889858454 CORE	5 O	O	0.0000	5
O	3.007364573	5.701784199	5.252959456 CORE	6 O	O	0.0000	6
O	10.166189021	10.049262906	4.491101001 CORE	7 O	O	0.0000	7
O	9.963752014	11.155506187	2.041879802 CORE	8 O	O	0.0000	8
O	8.583151685	7.791097446	0.435252457 CORE	9 O	O	0.0000	9
O	5.598027257	7.619862104	0.158789496 CORE	10 O	O	0.0000	10
O	4.869842607	4.276773657	1.445229385 CORE	11 O	O	0.0000	11
O	4.128868290	11.058282766	2.112267265 CORE	12 O	O	0.0000	12
O	2.204507522	5.003970002	1.781428594 CORE	13 O	O	0.0000	13
O	3.016596376	8.796728859	0.801744685 CORE	14 O	O	0.0000	14
O	3.616401501	1.143691671	2.772235088 CORE	15 O	O	0.0000	15
O	1.054903930	0.585613638	5.136891482 CORE	16 O	O	0.0000	16

O	2.664929326	7.442838112	3.137479674 CORE	17 O	O	0.0000	17
O	7.418489321	8.702379017	3.646812584 CORE	18 O	O	0.0000	18
O	5.908181409	1.742037168	0.034464996 CORE	19 O	O	0.0000	19
O	8.025208446	6.028456978	2.372256230 CORE	20 O	O	0.0000	20
O	7.592704463	10.854978126	5.294383810 CORE	21 O	O	0.0000	21
O	5.360332147	6.757080407	2.709279909 CORE	22 O	O	0.0000	22
O	7.004580386	1.392260702	5.940739879 CORE	23 O	O	0.0000	23
O	9.129254147	6.984022920	5.541580792 CORE	24 O	O	0.0000	24
O	5.639390883	5.738437872	5.178434796 CORE	25 O	O	0.0000	25
O	6.613181896	9.889114635	1.381856586 CORE	26 O	O	0.0000	26
O	4.321909228	9.290304054	4.119405511 CORE	27 O	O	0.0000	27
O	1.646721037	3.241921074	3.718559488 CORE	28 O	O	0.0000	28
Y	3.316470692	10.355672980	6.144494970 CORE	29 Y	Y	0.0000	29
Y	6.076115809	10.649768958	3.516805629 CORE	30 Y	Y	0.0000	30
Y	6.458646380	4.556611024	3.136404439 CORE	31 Y	Y	0.0000	31
Y	1.233146900	5.601252343	3.819192500 CORE	32 Y	Y	0.0000	32
Y	8.996302583	5.431587834	0.334606343 CORE	33 Y	Y	0.0000	33
Y	3.771370196	6.475693189	1.017587868 CORE	34 Y	Y	0.0000	34
Y	5.331311945	1.084962933	4.286903985 CORE	35 Y	Y	0.0000	35
Y	4.154027609	0.382739862	0.637297292 CORE	36 Y	Y	0.0000	36
Zr	3.202377757	3.198041417	2.351184904 CORE	37 Zr	Zr	0.0000	37
Zr	7.495354586	1.441613635	1.425524448 CORE	38 Zr	Zr	0.0000	38
Zr	2.734446388	9.591060363	2.728688637 CORE	39 Zr	Zr	0.0000	39
Zr	7.027761179	7.834839449	1.802937477 CORE	40 Zr	Zr	0.0000	40
Zr	4.364674099	4.221004423	5.958316508 CORE	41 Zr	Zr	0.0000	41
Zr	0.181599296	2.478248744	4.993837624 CORE	42 Zr	Zr	0.0000	42
Zr	4.282221063	7.219328587	4.473049257 CORE	43 Zr	Zr	0.0000	43
Zr	8.466600503	8.962601751	5.437784880 CORE	44 Zr	Zr	0.0000	44

end

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GM (40YSZ) Energy from NN is   -531.316980

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PBC   9.82134233   9.83330275   9.21561687   89.64767363   89.66340821   60.12136729

Zr	5.080955726	1.307107821	5.749119633 CORE	1 Zr Zr	0.0000	1
Zr	5.090984977	7.002751972	8.821017694 CORE	2 Zr Zr	0.0000	2
Zr	9.969539778	4.137788096	2.677449920 CORE	3 Zr Zr	0.0000	3
Zr	7.638077511	3.733021247	5.921260019 CORE	4 Zr Zr	0.0000	4
Zr	2.749381779	0.902403154	8.993042879 CORE	5 Zr Zr	0.0000	5
Zr	12.526688724	6.563523721	2.849580205 CORE	6 Zr Zr	0.0000	6
Zr	4.179399020	4.818264388	5.556499976 CORE	7 Zr Zr	0.0000	7
Zr	9.111819338	1.987747144	8.628155921 CORE	8 Zr Zr	0.0000	8
Zr	9.067628363	7.649344240	2.484311111 CORE	9 Zr Zr	0.0000	9
Y	1.644789703	2.293641876	5.906120581 CORE	10 Y	Y	0.0000	10
Y	11.476264689	7.989249788	8.977926723 CORE	11 Y	Y	0.0000	11

Y	6.533463490	5.124412366	2.834290109 CORE	12 Y	Y	0.0000	12
Y	8.443804788	0.252786345	5.607403129 CORE	13 Y	Y	0.0000	13
Y	8.453794506	5.948508670	8.679132143 CORE	14 Y	Y	0.0000	14
Y	3.511095682	3.083587223	2.535611334 CORE	15 Y	Y	0.0000	15
Y	7.347999535	7.329956179	5.573662258 CORE	16 Y	Y	0.0000	16
Y	12.280760433	4.499239273	8.645691118 CORE	17 Y	Y	0.0000	17
Y	7.337807334	1.634213344	2.501961020 CORE	18 Y	Y	0.0000	18
Y	10.774140498	6.279615324	5.928662355 CORE	19 Y	Y	0.0000	19
Y	5.885258102	3.449248150	9.000191440 CORE	20 Y	Y	0.0000	20
Y	0.942418348	0.584256828	2.856662156 CORE	21 Y	Y	0.0000	21
O	13.553869887	8.414718821	3.209763338 CORE	22 O	O	0.0000	22
O	4.210994037	5.168173946	3.310267573 CORE	23 O	O	0.0000	23
O	11.129100543	2.689370444	3.666785905 CORE	24 O	O	0.0000	24
O	11.134586793	2.456539139	8.277930189 CORE	25 O	O	0.0000	25
O	6.202062458	5.287367237	5.205985048 CORE	26 O	O	0.0000	26
O	3.096044268	0.917612698	2.053093759 CORE	27 O	O	0.0000	27
O	8.038850951	3.782438015	8.196824864 CORE	28 O	O	0.0000	28
O	7.079954631	1.530514600	0.178943535 CORE	29 O	O	0.0000	29
O	12.927681192	6.612938326	5.125336577 CORE	30 O	O	0.0000	30
O	8.216029071	3.870602753	3.841423841 CORE	31 O	O	0.0000	31
O	6.906907850	7.394598139	7.819004035 CORE	32 O	O	0.0000	32
O	6.196599507	5.520159395	0.594928942 CORE	33 O	O	0.0000	33
O	9.272811388	8.202330467	4.572644696 CORE	34 O	O	0.0000	34
O	4.384474301	5.371218287	7.644931180 CORE	35 O	O	0.0000	35
O	13.729624071	8.535854317	7.871558842 CORE	36 O	O	0.0000	36
O	5.791237926	3.073792065	6.756417561 CORE	37 O	O	0.0000	37
O	3.898416752	2.840246498	4.799556178 CORE	38 O	O	0.0000	38
O	8.787126836	5.671012973	1.727892804 CORE	39 O	O	0.0000	39
O	7.090054917	7.226181587	3.250653714 CORE	40 O	O	0.0000	40
O	3.722670312	2.719243867	0.137849822 CORE	41 O	O	0.0000	41
O	5.750824227	3.117556298	2.110347280 CORE	42 O	O	0.0000	42
O	6.896947259	1.698951719	4.747354058 CORE	43 O	O	0.0000	43
O	10.693564146	5.982361014	8.254108214 CORE	44 O	O	0.0000	44
O	3.327448249	1.039958652	6.913175957 CORE	45 O	O	0.0000	45
O	9.262810034	2.506288569	1.501263685 CORE	46 O	O	0.0000	46
O	8.665492025	5.584185228	6.281503017 CORE	47 O	O	0.0000	47
O	9.143622204	2.337466382	6.382038409 CORE	48 O	O	0.0000	48
O	11.139050775	8.384939389	6.738501450 CORE	49 O	O	0.0000	49
O	0.862193954	0.286755810	5.182196468 CORE	50 O	O	0.0000	50
O	10.680212701	5.903888011	3.685166713 CORE	51 O	O	0.0000	51
O	0.848641943	0.208526194	0.613059334 CORE	52 O	O	0.0000	52
O	11.785522267	4.529595991	1.675617172 CORE	53 O	O	0.0000	53
O	11.090483482	8.117745758	2.134192273 CORE	54 O	O	0.0000	54
O	13.104662054	6.701060556	0.769623934 CORE	55 O	O	0.0000	55

O	12.023050424	4.395268139	6.322810349 CORE	56 O	O	0.0000	56
O	9.099471120	7.998887066	0.238346959 CORE	57 O	O	0.0000	57

end

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8-P2

IS (GM) Energy from NN is -1492.124539

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PBC 9.89416880 17.80826343 10.96964204 89.54864308 101.73899789 89.20423358

O	8.348367250	1.317672119	0.566933859 CORE	1 O	O	0.0000	1
O	8.454719018	10.224580149	0.559107214 CORE	2 O	O	0.0000	2
O	-1.135570667	4.287939505	8.025238251 CORE	3 O	O	0.0000	3
O	-0.986637715	13.219826567	8.073934609 CORE	4 O	O	0.0000	4
Y	7.497964296	0.576907594	9.641738179 CORE	5 Y	Y	0.0000	5
Y	7.624537264	9.458044103	9.657598565 CORE	6 Y	Y	0.0000	6
Y	3.400784842	6.578976631	3.247039266 CORE	7 Y	Y	0.0000	7
Y	3.556570406	15.452559489	3.299362672 CORE	8 Y	Y	0.0000	8
Y	1.119867982	3.690801847	2.935800020 CORE	9 Y	Y	0.0000	9
Y	1.238602334	12.615399170	2.920552226 CORE	10 Y	Y	0.0000	10
Y	5.305270404	6.622944284	9.278499366 CORE	11 Y	Y	0.0000	11
Y	5.461596424	15.499037240	9.333802972 CORE	12 Y	Y	0.0000	12
O	0.301353727	1.404456675	6.561649437 CORE	13 O	O	0.0000	13
O	0.400989379	10.268742909	6.530038263 CORE	14 O	O	0.0000	14
O	4.411381498	2.687126201	7.461077870 CORE	15 O	O	0.0000	15
O	4.522126516	11.580398398	7.459374876 CORE	16 O	O	0.0000	16
Zr	0.089057951	6.508593119	1.103539571 CORE	17 Zr	Zr	0.0000	17
Zr	1.109348507	15.447879092	0.735268375 CORE	18 Zr	Zr	0.0000	18
O	8.310161920	2.863441739	6.015703883 CORE	19 O	O	0.0000	19
O	8.451569911	11.805940262	6.045936103 CORE	20 O	O	0.0000	20
Zr	-1.150011494	6.473237537	8.036774678 CORE	21 Zr	Zr	0.0000	21
Zr	-1.041369783	15.390743257	7.964120438 CORE	22 Zr	Zr	0.0000	22
O	7.017246434	5.522637804	3.864055306 CORE	23 O	O	0.0000	23
O	7.149259894	14.420856413	3.882542255 CORE	24 O	O	0.0000	24
O	2.584521440	4.473200233	6.881356856 CORE	25 O	O	0.0000	25
O	2.713161318	13.390913780	6.890340224 CORE	26 O	O	0.0000	26
Zr	6.777049777	3.560883682	7.665183684 CORE	27 Zr	Zr	0.0000	27
Zr	6.941662671	12.454170385	7.661439337 CORE	28 Zr	Zr	0.0000	28
O	7.617048758	2.835726674	9.698469490 CORE	29 O	O	0.0000	29
O	7.724578519	11.726266525	9.688555188 CORE	30 O	O	0.0000	30
O	4.992686200	5.546324661	1.668342583 CORE	31 O	O	0.0000	31
O	5.086778553	14.462439347	1.671735863 CORE	32 O	O	0.0000	32
Zr	8.216030703	0.590393505	6.085128071 CORE	33 Zr	Zr	0.0000	33
Zr	8.311724753	9.448863324	6.083507467 CORE	34 Zr	Zr	0.0000	34
O	1.776098111	4.259886045	10.495837762 CORE	35 O	O	0.0000	35

O	1.889295113	13.159363870	10.468854442 CORE	36 O	O	0.0000	36
O	3.347015820	17.805310867	3.380293390 CORE	37 O	O	0.0000	37
O	3.227633688	8.942018047	3.418422426 CORE	38 O	O	0.0000	38
O	6.804607358	5.858697033	7.473435048 CORE	39 O	O	0.0000	39
O	6.932472855	14.750684778	7.458635723 CORE	40 O	O	0.0000	40
O	1.000169002	1.432868114	2.878655795 CORE	41 O	O	0.0000	41
O	1.131737747	10.345979844	2.891460736 CORE	42 O	O	0.0000	42
Zr	0.010270300	6.679630388	4.615555602 CORE	43 Zr	Zr	0.0000	43
Zr	0.117893516	15.599509547	4.540030841 CORE	44 Zr	Zr	0.0000	44
O	-0.081471362	1.233918661	10.091370676 CORE	45 O	O	0.0000	45
O	0.019558229	10.200488948	10.077708869 CORE	46 O	O	0.0000	46
O	7.519459727	1.232410772	4.184320480 CORE	47 O	O	0.0000	47
O	7.641031358	10.161425693	4.204404042 CORE	48 O	O	0.0000	48
Zr	3.201496418	3.547202403	8.950247434 CORE	49 Zr	Zr	0.0000	49
Zr	3.336340362	12.424804417	8.952844431 CORE	50 Zr	Zr	0.0000	50
O	6.815772280	1.427904735	7.513147130 CORE	51 O	O	0.0000	51
O	6.943650735	10.322989429	7.499182044 CORE	52 O	O	0.0000	52
O	5.437893162	7.506110375	3.602885924 CORE	53 O	O	0.0000	53
O	5.586521068	16.397827785	3.598341650 CORE	54 O	O	0.0000	54
Zr	0.394968014	3.671562450	6.492047826 CORE	55 Zr	Zr	0.0000	55
Zr	0.537873397	12.617366729	6.492502210 CORE	56 Zr	Zr	0.0000	56
O	4.118512383	5.824621829	5.305746931 CORE	57 O	O	0.0000	57
O	4.262140967	14.737597578	5.337215632 CORE	58 O	O	0.0000	58
O	1.800562841	2.838526131	5.063930378 CORE	59 O	O	0.0000	59
O	1.922313621	11.749674252	5.081629308 CORE	60 O	O	0.0000	60
Zr	1.836023683	0.704951235	4.913398397 CORE	61 Zr	Zr	0.0000	61
Zr	1.902551242	9.619341528	4.917804938 CORE	62 Zr	Zr	0.0000	62
O	2.630487140	0.245151732	6.823558721 CORE	63 O	O	0.0000	63
O	2.750969560	9.191300207	6.818729731 CORE	64 O	O	0.0000	64
O	1.928873373	7.330259956	5.122526089 CORE	65 O	O	0.0000	65
O	2.053350432	16.216898593	5.109800820 CORE	66 O	O	0.0000	66
Zr	2.402708110	0.692001648	1.471352190 CORE	67 Zr	Zr	0.0000	67
Zr	2.547931758	9.538961627	1.475119242 CORE	68 Zr	Zr	0.0000	68
O	8.799210393	7.292118869	2.705717539 CORE	69 O	O	0.0000	69
O	8.698273563	3.032334015	2.487268431 CORE	70 O	O	0.0000	70
O	8.843128103	11.875815108	2.499690793 CORE	71 O	O	0.0000	71
Zr	8.902658189	0.558106639	2.575324522 CORE	72 Zr	Zr	0.0000	72
Zr	9.029660732	9.597398331	2.565219525 CORE	73 Zr	Zr	0.0000	73
O	3.386942326	4.156535791	3.377282111 CORE	74 O	O	0.0000	74
O	3.521066725	13.056472013	3.394940309 CORE	75 O	O	0.0000	75
O	2.794894090	1.434673566	9.379567091 CORE	76 O	O	0.0000	76
O	2.901973494	10.321975859	9.393486006 CORE	77 O	O	0.0000	77
O	-0.034212484	5.826783459	9.756711190 CORE	78 O	O	0.0000	78
O	0.061397039	14.782456495	9.871388208 CORE	79 O	O	0.0000	79

Zr	7.556913274	3.527655020	4.192616989 CORE	80 Zr Zr	0.0000	80
Zr	7.685678851	12.436156527	4.217031249 CORE	81 Zr Zr	0.0000	81
O	1.209018987	6.039501534	2.837019231 CORE	82 O O	0.0000	82
O	1.378528646	14.949905970	2.797283147 CORE	83 O O	0.0000	83
O	6.158179523	8.674525749	5.696657984 CORE	84 O O	0.0000	84
O	6.280570042	17.592458387	5.699785435 CORE	85 O O	0.0000	85
Zr	6.327924893	0.726370429	0.143958526 CORE	86 Zr Zr	0.0000	86
Zr	6.444721699	9.617984209	0.145602386 CORE	87 Zr Zr	0.0000	87
O	5.514312901	4.266857851	9.199719305 CORE	88 O O	0.0000	88
O	5.641771737	13.149693935	9.167856019 CORE	89 O O	0.0000	89
O	4.547790867	1.185838923	1.558677148 CORE	90 O O	0.0000	90
O	4.687191680	10.103247729	1.571525513 CORE	91 O O	0.0000	91
Zr	1.901339295	6.446656541	10.462089185 CORE	92 Zr Zr	0.0000	92
Zr	2.130202157	15.313824218	10.460657146 CORE	93 Zr Zr	0.0000	93
O	7.484038835	7.122651377	9.782162042 CORE	94 O O	0.0000	94
O	7.654161547	16.036551054	9.742969835 CORE	95 O O	0.0000	95
O	1.094004866	3.034147144	8.394042261 CORE	96 O O	0.0000	96
O	1.218595209	11.911833379	8.370616387 CORE	97 O O	0.0000	97
Zr	2.640418542	6.614915705	7.014584519 CORE	98 Zr Zr	0.0000	98
Zr	2.778586183	15.543096888	7.017699879 CORE	99 Zr Zr	0.0000	99
O	5.984394866	4.030513553	5.754752347 CORE	100 O O	0.0000	100
O	6.114039947	12.913158499	5.754769114 CORE	101 O O	0.0000	101
O	2.501213361	2.833425203	1.271153036 CORE	102 O O	0.0000	102
O	2.638700579	11.731391654	1.282089274 CORE	103 O O	0.0000	103
Zr	3.869251381	3.677551296	5.427536135 CORE	104 Zr Zr	0.0000	104
Zr	3.999587796	12.580496108	5.447927264 CORE	105 Zr Zr	0.0000	105
O	7.088359096	17.816247342	2.081575225 CORE	106 O O	0.0000	106
O	6.969093651	8.913802285	2.106795617 CORE	107 O O	0.0000	107
O	4.209816359	1.580002419	5.117596035 CORE	108 O O	0.0000	108
O	4.377119741	10.508720815	5.131266636 CORE	109 O O	0.0000	109
Zr	4.520488026	3.425448208	1.694383218 CORE	110 Zr Zr	0.0000	110
Zr	4.649890206	12.341322801	1.688939460 CORE	111 Zr Zr	0.0000	111
O	0.472864298	5.931962490	6.729567415 CORE	112 O O	0.0000	112
O	0.608616052	14.825543184	6.753022298 CORE	113 O O	0.0000	113
O	8.027596164	5.622508614	0.814623693 CORE	114 O O	0.0000	114
Zr	-0.284720461	3.710050567	10.001822427 CORE	115 Zr Zr	0.0000	115
Zr	-0.172735029	12.474601310	10.011347026 CORE	116 Zr Zr	0.0000	116
O	0.570142379	8.600747069	1.122661293 CORE	117 O O	0.0000	117
O	0.712032706	17.504887554	1.094860489 CORE	118 O O	0.0000	118
O	-0.856190893	8.580034708	8.003535296 CORE	119 O O	0.0000	119
O	-0.724571812	17.494843018	7.987594838 CORE	120 O O	0.0000	120
Zr	8.446072727	3.457920456	0.367205664 CORE	121 Zr Zr	0.0000	121
Zr	8.544330182	12.420066909	0.363963759 CORE	122 Zr Zr	0.0000	122
O	4.593592602	7.343079950	7.243724966 CORE	123 O O	0.0000	123

O	4.737325722	16.251083132	7.279664748 CORE	124 O	O	0.0000	124
O	6.299669686	2.964090307	0.283167244 CORE	125 O	O	0.0000	125
O	6.407039305	11.854697998	0.264049956 CORE	126 O	O	0.0000	126
Zr	6.729938875	6.760501904	2.116939241 CORE	127 Zr	Zr	0.0000	127
Zr	6.961904558	15.630630250	2.113405855 CORE	128 Zr	Zr	0.0000	128
O	-0.053613132	8.849585974	4.505101351 CORE	129 O	O	0.0000	129
O	0.103210799	17.786723333	4.551579686 CORE	130 O	O	0.0000	130
O	3.276829681	5.674207331	8.979695341 CORE	131 O	O	0.0000	131
O	3.423979838	14.568026028	8.979672758 CORE	132 O	O	0.0000	132
O	8.255161635	7.237520590	5.827818493 CORE	133 O	O	0.0000	133
O	8.392585660	16.137050567	5.846031393 CORE	134 O	O	0.0000	134
O	-0.306779574	4.576825656	4.588535625 CORE	135 O	O	0.0000	135
O	-0.174898430	13.490798901	4.573509442 CORE	136 O	O	0.0000	136
Zr	6.084325160	6.524745261	5.561676186 CORE	137 Zr	Zr	0.0000	137
Zr	6.226155060	15.444932037	5.559156871 CORE	138 Zr	Zr	0.0000	138
O	6.006668969	7.495304449	0.164125912 CORE	139 O	O	0.0000	139
O	6.099222721	16.413404117	0.169711078 CORE	140 O	O	0.0000	140
O	5.820127388	2.833890227	3.199440484 CORE	141 O	O	0.0000	141
O	5.962747330	11.754821350	3.177791140 CORE	142 O	O	0.0000	142
Zr	4.747176495	0.586156655	7.150150902 CORE	143 Zr	Zr	0.0000	143
Zr	4.866058066	9.497562857	7.129126303 CORE	144 Zr	Zr	0.0000	144
O	1.718921989	7.654076667	8.687331679 CORE	145 O	O	0.0000	145
O	1.844211761	16.550808062	8.712103722 CORE	146 O	O	0.0000	146
O	0.488941608	4.452455188	0.744573271 CORE	147 O	O	0.0000	147
O	0.632022553	13.354892696	0.716078534 CORE	148 O	O	0.0000	148
Zr	5.415659604	0.718068366	3.627661837 CORE	149 Zr	Zr	0.0000	149
Zr	5.518372259	9.651229039	3.615806685 CORE	150 Zr	Zr	0.0000	150
O	5.230497404	0.115130664	9.202192392 CORE	151 O	O	0.0000	151
O	5.344468313	9.019192461	9.184959328 CORE	152 O	O	0.0000	152
O	3.143164608	7.560713723	1.064063885 CORE	153 O	O	0.0000	153
O	3.065138255	16.333554557	1.024970989 CORE	154 O	O	0.0000	154
Zr	1.058523541	0.738971603	8.383671421 CORE	155 Zr	Zr	0.0000	155
Zr	1.177360187	9.637001975	8.356694108 CORE	156 Zr	Zr	0.0000	156
O	7.955315099	14.399977566	0.779183534 CORE	157 O	O	0.0000	157
O	8.898697323	16.249127172	2.820344753 CORE	158 O	O	0.0000	158

end
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TS   Energy from NN is   -1490.960452

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PBC 9.88793871 17.98097138 10.90046198 89.84691061 101.40600874 88.83021808

O	8.301266560	1.373523397	0.483763057 CORE	1 O	O	0.0000	1
O	8.505666911	10.325273640	0.552014574 CORE	2 O	O	0.0000	2
O	-1.030592015	4.319455139	8.023463452 CORE	3 O	O	0.0000	3
O	-0.885987211	13.368717326	8.027973098 CORE	4 O	O	0.0000	4

Y	7.579248861	0.567020102	9.572583970 CORE	5 Y	Y	0.0000	5
Y	7.800020120	9.499617326	9.602151694 CORE	6 Y	Y	0.0000	6
Y	3.497005599	6.638002261	3.248964743 CORE	7 Y	Y	0.0000	7
Y	3.645756948	15.641357313	3.221277301 CORE	8 Y	Y	0.0000	8
Y	1.229819937	3.733832469	2.920777734 CORE	9 Y	Y	0.0000	9
Y	1.377922475	12.677085615	2.877950184 CORE	10 Y	Y	0.0000	10
Y	5.403607860	6.655243199	9.205237808 CORE	11 Y	Y	0.0000	11
Y	5.617140869	15.724357247	9.163138563 CORE	12 Y	Y	0.0000	12
O	0.267797516	1.226867726	6.357694942 CORE	13 O	O	0.0000	13
O	0.374024808	10.381642152	6.470549891 CORE	14 O	O	0.0000	14
O	4.559429275	2.719982028	7.459669608 CORE	15 O	O	0.0000	15
O	4.858272630	11.778260774	7.633149121 CORE	16 O	O	0.0000	16
Zr	0.169036194	6.541283464	1.076871702 CORE	17 Zr	Zr	0.0000	17
Zr	0.984711226	15.703349317	0.858573322 CORE	18 Zr	Zr	0.0000	18
O	8.392916960	2.957803535	6.016364057 CORE	19 O	O	0.0000	19
O	8.431049886	12.100167271	5.914806223 CORE	20 O	O	0.0000	20
Zr	-1.051885507	6.479096359	8.029452962 CORE	21 Zr	Zr	0.0000	21
Zr	-0.912387450	15.538863189	7.971154583 CORE	22 Zr	Zr	0.0000	22
O	7.048684016	5.532357500	3.801782445 CORE	23 O	O	0.0000	23
O	7.576675623	14.821559808	4.060298373 CORE	24 O	O	0.0000	24
O	2.670313389	4.443899519	6.860241359 CORE	25 O	O	0.0000	25
O	2.842650632	13.354021953	6.846801487 CORE	26 O	O	0.0000	26
Zr	6.874563383	3.562947627	7.601741482 CORE	27 Zr	Zr	0.0000	27
Zr	7.001940012	12.569438727	7.626211343 CORE	28 Zr	Zr	0.0000	28
O	7.691834836	2.818479230	9.617937236 CORE	29 O	O	0.0000	29
O	7.962169881	11.730026450	9.646427298 CORE	30 O	O	0.0000	30
O	5.055397045	5.578096958	1.619239646 CORE	31 O	O	0.0000	31
O	5.073065925	14.632399302	1.631152106 CORE	32 O	O	0.0000	32
Zr	8.187797222	0.501668254	6.036636458 CORE	33 Zr	Zr	0.0000	33
Zr	8.316118838	9.412272203	6.004008303 CORE	34 Zr	Zr	0.0000	34
O	1.848412020	4.244019638	10.397563222 CORE	35 O	O	0.0000	35
O	2.010055111	13.302675914	10.379035021 CORE	36 O	O	0.0000	36
O	3.494488628	17.988006867	3.396651181 CORE	37 O	O	0.0000	37
O	3.413046227	9.054373703	3.474926733 CORE	38 O	O	0.0000	38
O	6.892367069	5.899127868	7.422457483 CORE	39 O	O	0.0000	39
O	7.039545071	14.944813018	7.401503299 CORE	40 O	O	0.0000	40
O	1.060282383	1.494240523	2.926149004 CORE	41 O	O	0.0000	41
O	1.308213851	10.366585184	2.848369710 CORE	42 O	O	0.0000	42
Zr	0.106603909	6.707973006	4.560945653 CORE	43 Zr	Zr	0.0000	43
Zr	0.297017654	15.619255005	4.721223497 CORE	44 Zr	Zr	0.0000	44
O	0.032568226	1.298260083	10.020402081 CORE	45 O	O	0.0000	45
O	0.205075697	9.990169201	10.046221723 CORE	46 O	O	0.0000	46
O	7.573380281	1.303243295	4.199903975 CORE	47 O	O	0.0000	47
O	7.700632325	10.191856190	4.172887267 CORE	48 O	O	0.0000	48

Zr	3.237378134	3.492110355	8.882905854 CORE	49 Zr Zr	0.0000	49	
Zr	3.277436010	12.424816984	8.846248635 CORE	50 Zr Zr	0.0000	50	
O	6.893396720	1.402834212	7.426118199 CORE	51 O O	0.0000	51	
O	7.104340022	10.424244776	7.431819187 CORE	52 O O	0.0000	52	
O	5.545613022	7.555202650	3.596489710 CORE	53 O O	0.0000	53	
O	5.711653545	16.498250369	3.537556825 CORE	54 O O	0.0000	54	
Zr	0.467272507	3.738838300	6.416645463 CORE	55 Zr Zr	0.0000	55	
Zr	0.522680065	12.576107582	6.408448749 CORE	56 Zr Zr	0.0000	56	
O	4.192997356	5.844484705	5.314327125 CORE	57 O O	0.0000	57	
O	4.283721475	14.882134933	5.284005191 CORE	58 O O	0.0000	58	
O	1.868716513	2.838706104	5.051869033 CORE	59 O O	0.0000	59	
O	2.030126834	11.787749977	5.018488789 CORE	60 O O	0.0000	60	
Zr	1.691590273	0.640470733	4.836134122 CORE	61 Zr Zr	0.0000	61	
Zr	1.957163656	9.674902448	4.847970221 CORE	62 Zr Zr	0.0000	62	
O	2.688870897	0.549993461	6.742837040 CORE	63 O O	0.0000	63	
O	2.860421874	9.474183853	6.738600637 CORE	64 O O	0.0000	64	
O	2.016151673	7.394339158	5.121114543 CORE	65 O O	0.0000	65	
O	2.147065758	16.455552526	5.253403060 CORE	66 O O	0.0000	66	
Zr	2.451081128	0.710356870	1.462868903 CORE	67 Zr Zr	0.0000	67	
Zr	2.675183400	9.598020637	1.424104998 CORE	68 Zr Zr	0.0000	68	
O	8.866141937	7.276224984	2.694096018 CORE	69 O O	0.0000	69	
O	8.759137610	2.979128732	2.446668579 CORE	70 O O	0.0000	70	
O	9.098088800	11.774973401	2.601672460 CORE	71 O O	0.0000	71	
Zr	8.910859099	0.808699020	2.459070247 CORE	72 Zr Zr	0.0000	72	
Zr	9.122002175	9.631755926	2.561415439 CORE	73 Zr Zr	0.0000	73	
O	3.480079742	4.205683122	3.363857753 CORE	74 O O	0.0000	74	
O	3.625223022	13.165381492	3.334140757 CORE	75 O O	0.0000	75	
O	2.854941497	1.387594434	9.357404309 CORE	76 O O	0.0000	76	
O	3.022173173	10.299890968	9.264217225 CORE	77 O O	0.0000	77	
O	0.060393373	5.859071386	9.746683584 CORE	78 O O	0.0000	78	
O	0.160422290	14.917672471	9.851620283 CORE	79 O O	0.0000	79	
Zr	7.601998149	3.559999242	4.186607574 CORE	80 Zr Zr	0.0000	80	
Zr	7.778872278	12.707850686	3.986391111 CORE	81 Zr Zr	0.0000	81	
O	1.319026980	6.082378256	2.811194491 CORE	82 O O	0.0000	82	
O	1.455555343	15.157580338	2.888441916 CORE	83 O O	0.0000	83	
O	6.234584831	8.688133194	5.730666977 CORE	84 O O	0.0000	84	
O	6.436346091	17.694838933	5.639403175 CORE	85 O O	0.0000	85	
Zr	6.323121414	0.684536576	0.147686042 CORE	86 Zr Zr	0.0000	86	
Zr	6.498283922	9.689560526	0.104853267 CORE	87 Zr Zr	0.0000	87	
O	5.656146211	4.325223194	9.141791843 CORE	88 O O	0.0000	88	
O	6.135003051	13.519792977	9.368573804 CORE	89 O O	0.0000	89	
O	4.617113743	1.151541428	1.547140273 CORE	90 O O	0.0000	90	
O	4.789957383	10.202427654	1.557980710 CORE	91 O O	0.0000	91	
Zr	2.008344439	6.455376313	10.376372301 CORE	92 Zr Zr	0.0000	92	

Zr	2.254419891	15.443258253	10.385605333 CORE	93 Zr Zr	0.0000	93
O	7.590883043	7.141465273	9.720278728 CORE	94 O O	0.0000	94
O	7.798059743	16.221790057	9.645676708 CORE	95 O O	0.0000	95
O	1.149775512	2.951476931	8.261368094 CORE	96 O O	0.0000	96
O	1.241154145	11.935827397	8.351294247 CORE	97 O O	0.0000	97
Zr	2.757758929	6.559461355	6.963132902 CORE	98 Zr Zr	0.0000	98
Zr	2.932220623	15.476869941	6.994825611 CORE	99 Zr Zr	0.0000	99
O	6.064796998	4.075357307	5.705879096 CORE	100 O O	0.0000	100
O	6.167668019	13.192774726	5.675568055 CORE	101 O O	0.0000	101
O	2.580037977	2.848202781	1.286616365 CORE	102 O O	0.0000	102
O	2.744337443	11.819418175	1.188485048 CORE	103 O O	0.0000	103
Zr	3.945798389	3.666467208	5.381517926 CORE	104 Zr Zr	0.0000	104
Zr	4.132164229	12.681518484	5.326048155 CORE	105 Zr Zr	0.0000	105
O	7.314416213	17.961807835	2.137157885 CORE	106 O O	0.0000	106
O	7.059719934	8.953205797	2.059571581 CORE	107 O O	0.0000	107
O	4.463695072	1.661251183	5.092294224 CORE	108 O O	0.0000	108
O	4.692346256	10.689518862	5.197765114 CORE	109 O O	0.0000	109
Zr	4.601914485	3.469125577	1.657901349 CORE	110 Zr Zr	0.0000	110
Zr	4.760350938	12.457127438	1.615137826 CORE	111 Zr Zr	0.0000	111
O	0.554865105	5.900984248	6.646355113 CORE	112 O O	0.0000	112
O	0.757483935	14.861671474	6.700836813 CORE	113 O O	0.0000	113
O	8.083273603	5.667426884	0.788078144 CORE	114 O O	0.0000	114
Zr	-0.190515478	3.639768921	9.945696151 CORE	115 Zr Zr	0.0000	115
Zr	-0.118303045	12.758960880	9.976334393 CORE	116 Zr Zr	0.0000	116
O	0.626104744	8.631231469	1.126505356 CORE	117 O O	0.0000	117
O	0.875185355	17.862441845	1.076847804 CORE	118 O O	0.0000	118
O	-0.752753704	8.565879375	7.902576280 CORE	119 O O	0.0000	119
O	-0.488759248	17.648062107	8.015913809 CORE	120 O O	0.0000	120
Zr	8.446495439	3.530844011	0.307114437 CORE	121 Zr Zr	0.0000	121
Zr	8.582583888	12.442547206	0.453353747 CORE	122 Zr Zr	0.0000	122
O	4.611560466	7.447274002	7.230732491 CORE	123 O O	0.0000	123
O	4.795842073	16.434848017	7.200139550 CORE	124 O O	0.0000	124
O	6.308557915	3.000619056	0.243964543 CORE	125 O O	0.0000	125
O	6.433251476	11.895617213	0.100123002 CORE	126 O O	0.0000	126
Zr	6.793141689	6.809684229	2.073875615 CORE	127 Zr Zr	0.0000	127
Zr	7.046299880	15.645478158	2.097278229 CORE	128 Zr Zr	0.0000	128
O	0.027162427	8.877342657	4.457515505 CORE	129 O O	0.0000	129
O	0.116869107	17.675964787	4.171576910 CORE	130 O O	0.0000	130
O	3.385645006	5.647646442	8.931491381 CORE	131 O O	0.0000	131
O	3.612348292	14.606017153	8.916132016 CORE	132 O O	0.0000	132
O	8.324012332	7.240905900	5.735230674 CORE	133 O O	0.0000	133
O	8.610314950	16.342787240	5.950394742 CORE	134 O O	0.0000	134
O	-0.251668689	4.601938504	4.492866400 CORE	135 O O	0.0000	135
O	0.036041038	13.551698847	4.499802345 CORE	136 O O	0.0000	136

Zr	6.177968617	6.544638667	5.513601427 CORE	137 Zr Zr	0.0000	137
Zr	6.273354042	15.559978928	5.555980545 CORE	138 Zr Zr	0.0000	138
O	6.046832081	7.557993298	0.127055229 CORE	139 O O	0.0000	139
O	6.251289680	16.502297355	0.159268834 CORE	140 O O	0.0000	140
O	5.915101850	2.844859807	3.111819160 CORE	141 O O	0.0000	141
O	6.035380580	11.873525666	3.155303572 CORE	142 O O	0.0000	142
Zr	4.761537157	0.620101226	7.064854980 CORE	143 Zr Zr	0.0000	143
Zr	4.965480006	9.612392025	7.141122532 CORE	144 Zr Zr	0.0000	144
O	1.828186329	7.659070965	8.567500024 CORE	145 O O	0.0000	145
O	2.073021785	16.668185879	8.604543403 CORE	146 O O	0.0000	146
O	0.532810406	4.457030184	0.740432261 CORE	147 O O	0.0000	147
O	0.636550260	13.533548141	0.771083646 CORE	148 O O	0.0000	148
Zr	5.484075120	0.688855619	3.575821332 CORE	149 Zr Zr	0.0000	149
Zr	5.624441061	9.721695474	3.595483796 CORE	150 Zr Zr	0.0000	150
O	5.285905866	0.103273645	9.111930704 CORE	151 O O	0.0000	151
O	5.517635435	9.061537582	9.139114044 CORE	152 O O	0.0000	152
O	3.256795728	7.606185719	1.114211778 CORE	153 O O	0.0000	153
O	3.135887020	16.542634739	1.011030504 CORE	154 O O	0.0000	154
Zr	1.124362860	0.695903455	8.263276582 CORE	155 Zr Zr	0.0000	155
Zr	1.248617309	9.652878681	8.271261585 CORE	156 Zr Zr	0.0000	156
O	7.610014634	13.692844052	1.755126035 CORE	157 O O	0.0000	157
O	8.985441301	16.034763008	1.594034917 CORE	158 O O	0.0000	158

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FS (2NN)   Energy from NN is   -1491.080126

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PBC   9.86779860   17.98045528   10.90451340   89.78895111   101.45115078   88.92518616

O	8.283371536	1.410354896	0.517965518 CORE	1 O O	0.0000	1
O	8.476767533	10.346078952	0.564153606 CORE	2 O O	0.0000	2
O	-1.040058879	4.337479708	8.023861803 CORE	3 O O	0.0000	3
O	-0.872161150	13.355526191	8.046549494 CORE	4 O O	0.0000	4
Y	7.560526476	0.587599137	9.594584251 CORE	5 Y Y	0.0000	5
Y	7.745246735	9.515411077	9.599295274 CORE	6 Y Y	0.0000	6
Y	3.477666699	6.637677101	3.246697852 CORE	7 Y Y	0.0000	7
Y	3.549468159	15.669925639	3.228370679 CORE	8 Y Y	0.0000	8
Y	1.228666911	3.744962064	2.920824178 CORE	9 Y Y	0.0000	9
Y	1.343551385	12.672660451	2.886067738 CORE	10 Y Y	0.0000	10
Y	5.370943964	6.670522928	9.208462789 CORE	11 Y Y	0.0000	11
Y	5.613774461	15.736744361	9.310299221 CORE	12 Y Y	0.0000	12
O	0.280864132	1.286424166	6.354288563 CORE	13 O O	0.0000	13
O	0.357279076	10.380717494	6.468498216 CORE	14 O O	0.0000	14
O	4.521340431	2.708365130	7.457516944 CORE	15 O O	0.0000	15
O	4.870989016	11.782935562	7.661115756 CORE	16 O O	0.0000	16
Zr	0.167183807	6.559254880	1.077379798 CORE	17 Zr Zr	0.0000	17

Zr	0.888040391	15.623918656	0.756571355 CORE	18 Zr	Zr	0.0000	18
O	8.355684380	2.962806105	6.030387773 CORE	19 O	O	0.0000	19
O	8.383288667	12.102087586	5.936545116 CORE	20 O	O	0.0000	20
Zr	-1.069858401	6.497601650	8.023389155 CORE	21 Zr	Zr	0.0000	21
Zr	-0.900791922	15.528492022	7.944031873 CORE	22 Zr	Zr	0.0000	22
O	7.033401356	5.555765017	3.824829276 CORE	23 O	O	0.0000	23
O	7.623225680	14.908937782	4.031433319 CORE	24 O	O	0.0000	24
O	2.642097167	4.433694622	6.863379843 CORE	25 O	O	0.0000	25
O	2.884043092	13.385107269	6.840052446 CORE	26 O	O	0.0000	26
Zr	6.847900594	3.567750390	7.610738237 CORE	27 Zr	Zr	0.0000	27
Zr	6.978860959	12.592926650	7.662849762 CORE	28 Zr	Zr	0.0000	28
O	7.664764155	2.843953133	9.624836655 CORE	29 O	O	0.0000	29
O	7.861048481	11.742493606	9.594995684 CORE	30 O	O	0.0000	30
O	5.033515084	5.583092154	1.625502361 CORE	31 O	O	0.0000	31
O	5.025157402	14.642044047	1.612526947 CORE	32 O	O	0.0000	32
Zr	8.182059994	0.521832132	6.058520683 CORE	33 Zr	Zr	0.0000	33
Zr	8.288905750	9.433192994	6.011408317 CORE	34 Zr	Zr	0.0000	34
O	1.829064498	4.264600466	10.406437978 CORE	35 O	O	0.0000	35
O	1.974856165	13.282330595	10.372776861 CORE	36 O	O	0.0000	36
O	3.431864956	17.993036379	3.392749593 CORE	37 O	O	0.0000	37
O	3.391529292	9.063464124	3.471223147 CORE	38 O	O	0.0000	38
O	6.856556908	5.907662605	7.429784438 CORE	39 O	O	0.0000	39
O	7.030087285	14.882812339	7.392883375 CORE	40 O	O	0.0000	40
O	1.047069762	1.505431153	2.912696363 CORE	41 O	O	0.0000	41
O	1.291166885	10.370308053	2.854346774 CORE	42 O	O	0.0000	42
Zr	0.096362181	6.716868017	4.576045762 CORE	43 Zr	Zr	0.0000	43
Zr	0.240129938	15.615936630	4.722471575 CORE	44 Zr	Zr	0.0000	44
O	-0.008706604	1.238882707	10.047654457 CORE	45 O	O	0.0000	45
O	0.162246061	10.180437251	10.042582846 CORE	46 O	O	0.0000	46
O	7.544781222	1.331263618	4.198167204 CORE	47 O	O	0.0000	47
O	7.671567391	10.199091747	4.179327944 CORE	48 O	O	0.0000	48
Zr	3.222350995	3.489764798	8.896569107 CORE	49 Zr	Zr	0.0000	49
Zr	3.277399907	12.462706007	8.838546342 CORE	50 Zr	Zr	0.0000	50
O	6.864477317	1.407862430	7.440389957 CORE	51 O	O	0.0000	51
O	7.071196678	10.406169845	7.427343870 CORE	52 O	O	0.0000	52
O	5.511159656	7.549244514	3.597753910 CORE	53 O	O	0.0000	53
O	5.638486373	16.492504251	3.518656517 CORE	54 O	O	0.0000	54
Zr	0.467122873	3.727996175	6.424814871 CORE	55 Zr	Zr	0.0000	55
Zr	0.488823772	12.583757048	6.401202996 CORE	56 Zr	Zr	0.0000	56
O	4.158754045	5.839067714	5.321315381 CORE	57 O	O	0.0000	57
O	4.272500859	14.929664416	5.279981682 CORE	58 O	O	0.0000	58
O	1.872881902	2.832045287	5.043966112 CORE	59 O	O	0.0000	59
O	2.012221862	11.801185475	5.020603388 CORE	60 O	O	0.0000	60
Zr	1.679601559	0.629620698	4.837522930 CORE	61 Zr	Zr	0.0000	61

Zr	1.945960377	9.687814346	4.860741434 CORE	62 Zr Zr	0.0000	62
O	2.677739089	0.481956886	6.743493951 CORE	63 O O	0.0000	63
O	2.828325695	9.494108234	6.759688997 CORE	64 O O	0.0000	64
O	2.004351691	7.407630962	5.129451308 CORE	65 O O	0.0000	65
O	2.113968335	16.431265390	5.209798698 CORE	66 O O	0.0000	66
Zr	2.413039421	0.669219340	1.452495597 CORE	67 Zr Zr	0.0000	67
Zr	2.662723456	9.619431011	1.435211909 CORE	68 Zr Zr	0.0000	68
O	8.843455285	7.285029045	2.696012771 CORE	69 O O	0.0000	69
O	8.734845955	3.037035648	2.461457876 CORE	70 O O	0.0000	70
O	9.055069695	11.771520549	2.625859217 CORE	71 O O	0.0000	71
Zr	8.892776541	0.891811251	2.497189196 CORE	72 Zr Zr	0.0000	72
Zr	9.085398531	9.639946804	2.573926116 CORE	73 Zr Zr	0.0000	73
O	3.463755786	4.209779804	3.361664674 CORE	74 O O	0.0000	74
O	3.567765566	13.242044760	3.329448784 CORE	75 O O	0.0000	75
O	2.835670028	1.385473572	9.368457408 CORE	76 O O	0.0000	76
O	3.001005564	10.319597927	9.276659619 CORE	77 O O	0.0000	77
O	0.038633487	5.873450163	9.754760155 CORE	78 O O	0.0000	78
O	0.089954689	14.870459568	9.893746797 CORE	79 O O	0.0000	79
Zr	7.566106783	3.586546688	4.206447202 CORE	80 Zr Zr	0.0000	80
Zr	7.714968392	12.740455923	3.986025493 CORE	81 Zr Zr	0.0000	81
O	1.306262439	6.092682403	2.817876873 CORE	82 O O	0.0000	82
O	1.277053434	15.212753689	2.834610098 CORE	83 O O	0.0000	83
O	6.188748278	8.705428897	5.708234449 CORE	84 O O	0.0000	84
O	6.408701127	17.696836854	5.634151962 CORE	85 O O	0.0000	85
Zr	6.303783783	0.677991566	0.169239531 CORE	86 Zr Zr	0.0000	86
Zr	6.471505825	9.695894163	0.116905164 CORE	87 Zr Zr	0.0000	87
O	5.609789359	4.326796178	9.141204068 CORE	88 O O	0.0000	88
O	6.071361281	13.534009043	9.405361218 CORE	89 O O	0.0000	89
O	4.623859012	1.132024867	1.575288285 CORE	90 O O	0.0000	90
O	4.775301893	10.199301387	1.549514207 CORE	91 O O	0.0000	91
Zr	1.994233083	6.470567814	10.382980474 CORE	92 Zr Zr	0.0000	92
Zr	2.158220777	15.444616575	10.365063546 CORE	93 Zr Zr	0.0000	93
O	7.553960375	7.151697171	9.720591791 CORE	94 O O	0.0000	94
O	7.835202835	16.296601907	9.517129726 CORE	95 O O	0.0000	95
O	1.124170875	2.951448541	8.291255286 CORE	96 O O	0.0000	96
O	1.260923933	11.951739536	8.311470749 CORE	97 O O	0.0000	97
Zr	2.731845387	6.553931432	6.969741430 CORE	98 Zr Zr	0.0000	98
Zr	2.951345773	15.504572450	6.993031560 CORE	99 Zr Zr	0.0000	99
O	6.034826014	4.080696642	5.717102577 CORE	100 O O	0.0000	100
O	6.151151133	13.225945252	5.612854926 CORE	101 O O	0.0000	101
O	2.573013889	2.828639959	1.274291637 CORE	102 O O	0.0000	102
O	2.749136462	11.828000120	1.245597041 CORE	103 O O	0.0000	103
Zr	3.924539586	3.648949713	5.384849345 CORE	104 Zr Zr	0.0000	104
Zr	4.116418778	12.712466564	5.282343547 CORE	105 Zr Zr	0.0000	105

O	7.368119016	17.850388969	2.155972297 CORE	106 O	O	0.0000	106
O	7.030284188	8.955457791	2.072602132 CORE	107 O	O	0.0000	107
O	4.455561448	1.639421847	5.089991816 CORE	108 O	O	0.0000	108
O	4.630224168	10.694489788	5.221736351 CORE	109 O	O	0.0000	109
Zr	4.582798644	3.461801508	1.663135226 CORE	110 Zr	Zr	0.0000	110
Zr	4.754076718	12.464456719	1.617551743 CORE	111 Zr	Zr	0.0000	111
O	0.547565174	5.915403187	6.661159365 CORE	112 O	O	0.0000	112
O	0.751149709	14.844324088	6.676551547 CORE	113 O	O	0.0000	113
O	8.061060811	5.679386244	0.786654062 CORE	114 O	O	0.0000	114
Zr	-0.205820129	3.689942440	9.956543212 CORE	115 Zr	Zr	0.0000	115
Zr	-0.127878892	12.625854270	9.972812177 CORE	116 Zr	Zr	0.0000	116
O	0.624784887	8.648507471	1.110122897 CORE	117 O	O	0.0000	117
O	0.744269856	17.760940053	1.154158501 CORE	118 O	O	0.0000	118
O	-0.746986836	8.586937313	7.940077875 CORE	119 O	O	0.0000	119
O	-0.511137846	17.706004009	7.968725571 CORE	120 O	O	0.0000	120
Zr	8.420340064	3.550229630	0.307924878 CORE	121 Zr	Zr	0.0000	121
Zr	8.526640697	12.460525969	0.492106693 CORE	122 Zr	Zr	0.0000	122
O	4.589412343	7.456772185	7.224654226 CORE	123 O	O	0.0000	123
O	4.811157278	16.431607256	7.249194114 CORE	124 O	O	0.0000	124
O	6.282565165	3.007460674	0.250145189 CORE	125 O	O	0.0000	125
O	6.402215364	11.904297511	0.117722725 CORE	126 O	O	0.0000	126
Zr	6.771358516	6.816765938	2.082430217 CORE	127 Zr	Zr	0.0000	127
Zr	6.928465018	15.597754920	2.034444028 CORE	128 Zr	Zr	0.0000	128
O	0.018773392	8.881158157	4.460917854 CORE	129 O	O	0.0000	129
O	0.066754503	17.701580224	4.202109017 CORE	130 O	O	0.0000	130
O	3.357530218	5.654824224	8.928041171 CORE	131 O	O	0.0000	131
O	3.572095481	14.636910769	8.936827871 CORE	132 O	O	0.0000	132
O	8.296171890	7.261066470	5.764887787 CORE	133 O	O	0.0000	133
O	8.564928059	16.355459651	5.976045515 CORE	134 O	O	0.0000	134
O	-0.244354339	4.606282710	4.517213997 CORE	135 O	O	0.0000	135
O	0.002839573	13.544879237	4.505594756 CORE	136 O	O	0.0000	136
Zr	6.130389102	6.563262019	5.530648936 CORE	137 Zr	Zr	0.0000	137
Zr	6.272179727	15.561200692	5.552503916 CORE	138 Zr	Zr	0.0000	138
O	6.029102000	7.558759067	0.133322638 CORE	139 O	O	0.0000	139
O	6.100725350	16.557082032	0.160777887 CORE	140 O	O	0.0000	140
O	5.898353395	2.858078285	3.118794366 CORE	141 O	O	0.0000	141
O	5.934718486	11.855434217	3.221291915 CORE	142 O	O	0.0000	142
Zr	4.757590522	0.602479572	7.079520958 CORE	143 Zr	Zr	0.0000	143
Zr	4.941494895	9.630656263	7.149059130 CORE	144 Zr	Zr	0.0000	144
O	1.818625254	7.681347060	8.585453139 CORE	145 O	O	0.0000	145
O	1.964888708	16.647906709	8.583427776 CORE	146 O	O	0.0000	146
O	0.531395327	4.472229465	0.747520787 CORE	147 O	O	0.0000	147
O	0.628105651	13.445268236	0.774978517 CORE	148 O	O	0.0000	148
Zr	5.495872604	0.665371859	3.585912877 CORE	149 Zr	Zr	0.0000	149

Zr	5.591350134	9.718690810	3.628149092 CORE	150 Zr Zr	0.0000	150
O	5.270505757	0.124785213	9.154188426 CORE	151 O O	0.0000	151
O	5.483711166	9.066390418	9.152889560 CORE	152 O O	0.0000	152
O	3.234134324	7.631198467	1.093709632 CORE	153 O O	0.0000	153
O	3.079786695	16.541269293	1.001754759 CORE	154 O O	0.0000	154
Zr	1.103301714	0.697114953	8.265207524 CORE	155 Zr Zr	0.0000	155
Zr	1.240678643	9.673689936	8.272233682 CORE	156 Zr Zr	0.0000	156
O	7.458716401	13.582206848	1.894765573 CORE	157 O O	0.0000	157
O	8.675488835	15.699671083	0.927036631 CORE	158 O O	0.0000	158

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